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MODELING THE FATE OF TOXIC ORGANIC MATERIALS IN AQUATIC ENVIRONMENTS

by

Richard A. Park, Christopher I. Connolly, James R. Albanese,
Lenore S. Clesceri, George W. Heitzman, Harry H. Herbrandson,
Barry H. Indyke, Joseph R. Loehe, Sydney Ross,
Dineshchand D. Sharma, and William W. Shuster

Center for Ecological Modeling
Rensselaer Polytechnic Institute
Troy, New York 12181

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Project Officer

Lawrence A. Burns
Environmental Systems Branch
Environmental Research Laboratory
Athens, Georgia 30613

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
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16. ABSTRACT

Documentation is given for PEST, a dynamic simulation model for evaluating the fate of toxic organic materials (TOM) in freshwater environments. PEST represents the time-varying concentration (in ppm) of a given TOM in each of as many as 16 carrier compartments; it also computes the percent distribution and half life of the TOM in each of the carriers. Possible carriers include phytoplankton, macrophytes, zooplankton, waterbugs, zoobenthos, fish, particulate organic matter, floating organic matter, clay, and water (with TOM in the dissolved phase). PEST simulates TOM degradation by hydrolysis, oxidation, photolysis, microbial metabolism, and biotransformation by higher organisms; it simulates TOM transfer by solution, volatilization, sorption, absorption onto gills, consumption, excretion, defecation, biodeposition, mortality, and throughflow. These are subject to time-varying environmental factors such as pH, temperature, dissolved oxygen, wind, solar radiation, and biomass and condition of organisms. The model has been verified with process-level laboratory data and with ecosystem-level site data. The site data for fish ponds in Missouri and Israel and a reservoir in Iowa constitute prototype data sets that can be used to evaluate other compounds.

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FOREWORD

Environmental protection efforts are increasingly directed toward preventing adverse health and ecological effects associated with specific compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact and control of environmental contaminants, the Environmental Systems Branch studies complexes of environmental processes that control the transport, transformation, degradation, fate, and impact of pollutants or other materials in soil and water and develops models for assessing exposure to chemical contaminants.

Concern about environmental exposure to synthetic organic compounds has increased the need for techniques to predict the behavior of chemicals entering the environment as a result of the manufacture, use, and disposal of commercial products. In response to this need, a number of mathematical models have been developed to provide information about the fate of these materials as an aid to environmental researchers, planners, and managers. This report describes PEST, a dynamic simulation model for evaluating the fate of toxic organic materials in freshwater environments that provides a particularly detailed analysis of bioaccumulation.

David W. Duttweiler
Director
Environmental Research Laboratory
Athens, Georgia

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ABSTRACT

Documentation is given for PEST, a dynamic simulation model for evaluating the fate of toxic organic materials (TOM) in freshwater aquatic environments. PEST represents the time-varying concentration (in ppm) of a given TOM in each of as many as sixteen carrier compartments; it also computes the percent distribution and half life of the TOM in each of the carriers. Possible carriers include phytoplankton, macrophytes, zooplankton, waterbugs, zoobenthos, fish, particulate organic matter, floating organic matter, clay, and water (with TOM in the dissolved phase).

PEST simulates TOM degradation by hydrolysis, oxidation, photolysis, microbial metabolism, and biotransformation by higher organisms; it simulates TOM transfer by solution, volatilization, sorption, absorption onto gills, consumption, excretion, defecation, biodeposition, mortality, and throughflow. These are subject to time-varying environmental factors such as pH, temperature, dissolved oxygen, wind, solar radiation, and biomass and condition of organisms.

The model has been verified with process-level laboratory data and with ecosystem-level site data. The site data for fish ponds in Missouri and Israel and a reservoir in Iowa constitute prototype data sets that can be used to evaluate other compounds.

PEST is an interactive, user-oriented model with twelve commands. The user can edit parameters and driving variables, display process-response curves for all combinations of processes and driving variables, run a simulation for any length of time, print any or all state-variable results, debug loadings and rates during the simulation, tabulate the results, obtain line-printer and graphics-device plots, dump COMMON block contents, and access an extensive HELP file.

The model is written in standard FORTRAN IV and will run in 22k on a PDP11 with overlaying. It has also been tested on an IBM3033. The program is well structured and highly modular and is easy to understand. System-dependent features are restricted to two optional subroutines: one which handles operations such as file numbering and time calls and one which provides an interface to graphics terminals and plotters. Instructions are

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EPA-287 (Cin.)
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given for converting the program and data files from the distribution tape to the user's computer installation.

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TYPING GUIDE SHEET
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TOP OF IMAGE AREA
DROPPED HEAD: BEGIN SECTIONS HERE

CONTENTS

FOREWORD. iii
ABSTRACT. iv
FIGURES ix
TABLES. xiv
ACKNOWLEDGEMENTS. xv

1. INTRODUCTION. 1

    RELATIONSHIP TO OTHER MODELS. 1
    CHARACTERISTICS OF MODEL. 2

2. PROCESS EQUATIONS AND PARAMETERIZATION. 7

    HYDROLYSIS. 7
        Verification. 13
    OXIDATION 15
    PHOTOLYSIS. 16
        Verification. 21
    VOLATILIZATION. 24
        Gas-phase Mass Transfer Coefficient 26
        Liquid-phase Mass Transfer Coefficient. 28
        Verification. 30
    SOLUTION. 31
    MICROBIAL METABOLISM. 32
    SORPTION. 40
    GILL SORPTION 41
    CONSUMPTION 44
        Ingestion 45
    BIOTRANSFORMATION 48

3. DATA REQUIREMENTS 51

    COMPOUND-SPECIFIC PARAMETERS. 51
        1. Hydrolysis. 51
        2. Oxidation 52
        3. Photolysis. 52
        4. Volatilization. 52
        5. Solution. 52
        6. Microbial Degradation 52
        7. Sorption. 53
        8. Bioaccumulation 53

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

SITE-SPECIFIC CONSTANTS AND DRIVING VARIABLES . . 53
ORGANISM-SPECIFIC PARAMETERS. 54

4. VERIFICATION. 57

PARATHION IN ISRAELI FISHPONDS. 58
PENTACHLOROPHENOL IN MISSOURI FISHPONDS 61
DIELDRIN IN AN IOWA RESERVOIR 63

5. USER'S MANUAL 68

LOGON 68
  Example 68
EDIT. 68
  Syntax. 68
  Examples. 69
START 69
  Syntax. 69
  Example 70
PRINT 70
  Syntax. 71
  Example 71
DEBUG 71
  Syntax. 72
  Example 72
TABULATE. 73
  Syntax. 73
  Example 73
PLOT. 73
  Syntax. 74
  Example 74
DISPLAY 75
  Syntax. 75
  Example 75
DUMP. 76
  Syntax. 76
  Example 76
HELP. 77
  Syntax. 77
  Example 77
QUIT. 78
  Syntax. 78
  Example 78

6. PROGRAMMER'S GUIDE. 79

INTRODUCTION. 79
FILE UNITS. 79
COMMON BLOCKS 81
BUILDING A MODEL. 82

7. REFERENCES. 84

TYPING GUIDE SHEET
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TOP OF IMAGE AREA
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BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

BEGIN FIRST LINE OF TEXT HERE
TYPING GUIDE SHEET
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TOP OF IMAGE AREA
DROPPED HEAD; BEGIN SECTIONS HERE

APPENDICES. 92

A Parameters and Loadings used in Simulation of Pond A-7, Dor, Israel. 92

B Parameters and Loadings used in Simulation of Treatment-3 Ponds, Columbia, Missouri. 112

C Loadings used in Simulation of Treatment-2 Ponds, Columbia, Missouri 131

D Parameters and Loadings used in Simulation of Coralville Reservoir, Iowa 135

GLOSSARY OF PARAMETERS AND VARIABLES. 156

INDEX 162

6-1/2"
9-1/8"
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3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD, BEGIN SECTIONS HERE

FIGURES

Number Page
1 Compartments in the PEST model. 3
2 PEST process flow chart 5
3a Hydrolysis of parathion 9
3b Hydrolysis of pentachlorophenol 10
3c Hydrolysis of methoxychlor. 10
3d Hydrolysis of 2,4-D 11
4a Sensitized photolysis of methoxychlor 23
4b Unsensitized photolysis of methoxychlor 23
4c Photolysis of pentachlorophenol 24
5 Two-film model of volatilization from the surface of water. 25
6 Volatilization of a hypothetical liquid-phase control compound. 30
7 Malathion remaining vs. incubation time 34
8 Effect of dissolved oxygen on microbial degradation of pentachlorophenol. 35
9 Effect of pH on microbial degradation of pentachlorophenol 36
10 Effect of temperature on microbial degradation of pentachlorophenol. 37
11 Relation between the concentration of methoxychlor in a fish and time 45
12 Relationship between BTRANS (g transformed/g organism/day) and TOM concentration (g TOM/g) . . . 50

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

13a Comparison of predicted and observed concentrations of Parathion in dissolved phase in Pond A-7, Dor, Israel 58

13b Comparison of predicted and observed concentrations of Parathion in zooplankton in Pond A-7, Dor, Israel. 59

13c Comparison of predicted and observed concentrations of Parathion in carp in Pond A-7, Dor, Israel. 59

13d Comparison of predicted and observed concentrations of Parathion in *Tilapia* in Pond A-7, Dor, Israel. 60

13e Comparison of predicted and observed concentrations of Parathion in silver carp in Pond A-7, Dor, Israel 60

14a Comparison of predicted and observed concentrations of Pentachlorophenol in dissolved phase in Treatment-3 ponds, Columbia, Missouri . . . 61

14b Predicted concentrations of Pentachlorophenol in clay and particulate organic material in Treatment-3 ponds, Columbia, Missouri. 62

14c Predicted concentrations of Pentachlorophenol in phytoplankton and zooplankton in Treatment-3 ponds, Columbia, Missouri. 62

14d Predicted and observed concentrations of Pentachlorophenol in large-mouth bass in Treatment-3 ponds, Columbia, Missouri. 63

15a Comparison of predicted and observed concentrations of Pentachlorophenol in dissolved phase in Treatment-2 ponds, Columbia, Missouri 64

15b Comparison of predicted and observed concentrations of Pentachlorophenol in bluegills in Treatment-2 ponds, Columbia, Missouri 64

15c Comparison of predicted and observed concentrations of Pentachlorophenol in large-mouth bass in Treatment-2 ponds, Columbia, Missouri. . . . 65

15d Comparison of predicted and observed concentrations of Pentachlorophenol in channel catfish in Treatment-2 ponds, Columbia, Missouri . . 65

16a Comparison of predicted and observed concentrations of Dieldrin in dissolved phase in Coralville Reservoir, Iowa from 1968 to 1977 66

16b Comparison of predicted and observed concentrations of Dieldrin in carp in Coralville Reservoir, Iowa 67

16c Comparison of predicted and observed concentrations of Dieldrin in the dissolved phase in Coralville Reservoir, Iowa 67

A1 Temperature loading used in simulation of Pond A-7, Dor, Israel 107

A2 pH loading used in simulation of Pond A-7, Dor, Israel 107

A3 Dissolved oxygen loading used in simulation of Pond A-7, Dor, Israel 108

A4 Wind velocity loading used in simulation of Pond A-7, Dor, Israel 108

A5 Solar radiation loading used in simulation of Pond A-7, Dor, Israel 109

A6 Phytoplankton biomass used in simulation of Pond A-7, Dor, Israel 109

A7 Zooplankton biomass used in simulation of Pond A-7, Dor, Israel 110

A8 Water bug biomass used in simulation of Pond A-7, Dor, Israel 110

A9 Carp biomass used in simulation of Pond A-7, Dor, Israel 111

B1 Temperature loading used in simulation of Treatment-3 ponds, Columbia, Missouri 127

B2 pH loading used in simulation of Treatment-3 ponds, Columbia, Missouri 127

B3 Dissolved oxygen loading used in simulation of Treatment-3 ponds, Columbia, Missouri 128

B4 Wind velocity loading used in simulation of Treatment-3 ponds, Columbia, Missouri 128

TYPING GUIDE SHEET
EPA-287 (Cin.)
(4-76)

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD, BEGIN SECTIONS HERE

B5 Solar radiation loading used in simulation of Treatment-3 ponds, Columbia, Missouri. 129
B6 Phytoplankton biomass used in simulation of Treatment-3 ponds, Columbia, Missouri. 129
B7 Zooplankton biomass used in simulation of Treatment-3 ponds, Columbia, Missouri 130
B8 Bluegill biomass used in simulation of Treatment-3 ponds, Columbia, Missouri 130
C1 Temperature loadings used in simulation of Treatment-2 ponds, Columbia, Missouri 131
C2 pH loadings used in simulation of Treatment-2 ponds, Columbia, Missouri 131
C3 Dissolved oxygen loadings used in simulation of Treatment-2 ponds, Columbia, Missouri. 132
C4 Phytoplankton biomass used in simulation of Treatment-2 ponds, Columbia, Missouri 132
C5 Zooplankton biomass used in simulation of Treatment-2 ponds, Columbia, Missouri 133
C6 Bluegill biomass used in simulation of Treatment-2 ponds, Columbia, Missouri 133
C7 Pentachlorophenol loadings used in simulation of Treatment-2 ponds, Columbia, Missouri. 134
D1 Temperature loadings used in simulation of Coralville Reservoir, Iowa. 150
D2 pH loadings used in simulation of Coralville Reservoir, Iowa. 150
D3 Dissolved oxygen loadings used in simulation of Coralville Reservoir, Iowa 151
D4 Wind loadings used in simulation of Coralville Reservoir, Iowa. 151
D5 Particulate organic matter loadings used in simulation of Coralville Reservoir, Iowa. 152
D6 Clay loadings used in simulation of Coralville Reservoir, Iowa. 152

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

D7 Phytoplankton biomass used in simulation of Coralville Reservoir, Iowa 153

D8 Zooplankton biomass used in simulation of Coralville Reservoir, Iowa 153

D9 Carp biomass used in simulation of Coralville Reservoir, Iowa. 154

D10 Water flow loadings used in simulation of Coralville Reservoir, Iowa. 154

D11 Dieldrin loadings used in simulation of Coralville Reservoir, Iowa. 155

EPA-287 (Cin.)
(4-76)

BEGIN FIRST LINE OF TEXT HERE
TYPING GUIDE SHEET
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD; BEGIN SECTIONS HERE

TABLES

Number Page

1 STATE VARIABLE EQUATIONS. 3

2 PARAMETERS (1/M day) FOR SELECTED COMPOUNDS . . . 9

3 COMPARISON OF PEST HYDROLYSIS HALF-LIVES WITH LITERATURE VALUES FOR VARIATIONS IN pH AT CONSTANT TEMPERATURE. 14

4 COMPARISON OF THE SOLAR INTENSITY BREAKDOWN IN PEST WITH THE RESULTS OBTAINED BY ZEPP AND CLINE (1977). 18

5 ATTENUATION COEFFICIENTS (AS PRESENTED BY HAUTALA, 1978). 19

6 ATTENUATION SENSITIVITY ANALYSIS OF PENTACHLOROPHENOL UNDER MIDSUMMER SUN. 20

7 COMPARISON OF PEST PHOTOLYSIS HALF-LIVES WITH LITERATURE VALUES 22

8 CALCULATED HENRY'S LAW CONSTANTS. 27

9 LE BAS ADDITIVE VOLUMES TO CALCULATE LIQUID MOLAL VOLUME (cc/g mole). 27

10 CALCULATED OR OBSERVED MOLAL VOLUMES FOR SELECTED COMPOUNDS. 28

11 VERIFICATION OF TEMPERATURE CORRECTION. 29

12 LIQUID-PHASE MASS TRANSFER COEFFICIENTS AT 25°C. 29

13 COMPARISON OF PEST VOLATILIZATION RATES WITH LITERATURE VALUES 31

BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
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3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

SECTION 1

INTRODUCTION

RELATIONSHIP TO OTHER MODELS

The PEST model has been under development for the past four years in response to the need for a detailed, chemically- and biologically-realistic model to predict the fate of toxic organic materials in natural aquatic environments. As such, its development has paralleled that of several other fate models; however, each model has its particular emphasis, and PEST fulfills a need for detail and biologic realism that is not addressed by other models (Park et al., 1980; Albanese et al. 1981).

PEST can be considered an evaluative model in the sense of Lassiter (1975). As such, it is intended to be used primarily to indicate the relative importance of the various processes under well defined environmental conditions and to determine the environmental compatibility of particular organic materials. Many of the demands placed on the EPA relative to evaluating new materials can be answered through the expediency of such a process-oriented evaluative model. The model can also assist in the extrapolation of data from laboratory experiments and microcosms to natural environments (Park, Indyke and Heitzman, in press).

PEST is often compared with the EXAMS model; both are components of the fate modeling program of the Environmental Systems Branch of the Athens Environmental Research Laboratory. EXAMS was developed as an in-house effort (Lassiter, Baughman, and Burns, 1978; Baughman and Burns, 1979; Burns, Cline and Lassiter, in press). EXAMS differs from PEST in that: 1) it partitions the chemical into ionic species; 2) it represents bioaccumulation as a bioconcentration factor for the ecosystem; and 3) it is a steady-state model. EXAMS is designed for use as a quick screening tool, while PEST provides a more detailed analysis, especially with respect to bioaccumulation.

A similar model, based in part on the SRI model (Smith et al., 1977), was programmed by Schnoor et al (1979). It represents non-steady state and considers bioaccumulation in several fish types; therefore it comes somewhat closer to the concept of PEST. A model developed at DOW Chemical Company

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(Neely and Blau, 1977; Branson, 1978) is simpler in concept but does distinguish between uptake and depuration in fish.

The SERATRA model (Onishi, and Wise, 1979) is characterized by good hydrodynamic resolution. Its chemical and biological realism is less than PEST, but it is probably better than PEST in representing physical transport of toxic organic materials in riverine and estuarine environments.

Another group of fate models emphasize bioaccumulation, but ignore chemical processes. Thomann (1978) models bioaccumulation in relation to size of organism. Weininger (1978) considers detailed bioenergetics in simulating the uptake of polychlorinated biphenyls (PCBs) by lake trout; his approach is similar to that used in modeling bioaccumulation in PEST, although the extreme lipophilic nature of PCBs permits some simplifications that are not taken in PEST.

Each of these models serves a specific purpose. However, only PEST combines detailed chemical kinetics and bioenergetics to permit examination and evaluation of the behavior of toxic organic materials in the context of the entire aquatic ecosystem. Of course, use of such a complex model requires an understanding of the many assumptions and parameters, as well as a knowledge of the mechanics of the program. The purpose of this report is to acquaint the potential user with the details of PEST so that the model can be used both easily and wisely.

CHARACTERISTICS OF MODEL

PEST is capable of simulating the time-varying concentration of a toxic organic material (TOM) in each of as many as sixteen carrier compartments. The sixteen state variables can be parameterized to represent a variety of TOM-carrier associations typical of aquatic ecosystems (for example Figure 1).

The state-variable equations are ordinary differential equations with source and sink terms for the various processes that result in additions to, and losses from, the carriers (Table 1). Broad categories include TOM in: plants, such as phytoplankton and macrophytes; animals, such as zooplankton, waterbugs, zoobenthos, and fish (different species and/or age classes); dissolved phase, either in the water column or in interstitial water; particulate organic matter, either suspended or as bottom sediment; floating organic matter, usually as a surface film; and clay, either suspended or as bottom sediment.

The source and sink terms for the state variables are represented by process equations. Most of the process equations are non-linear, and many involve several different environmental factors (Figure 2).

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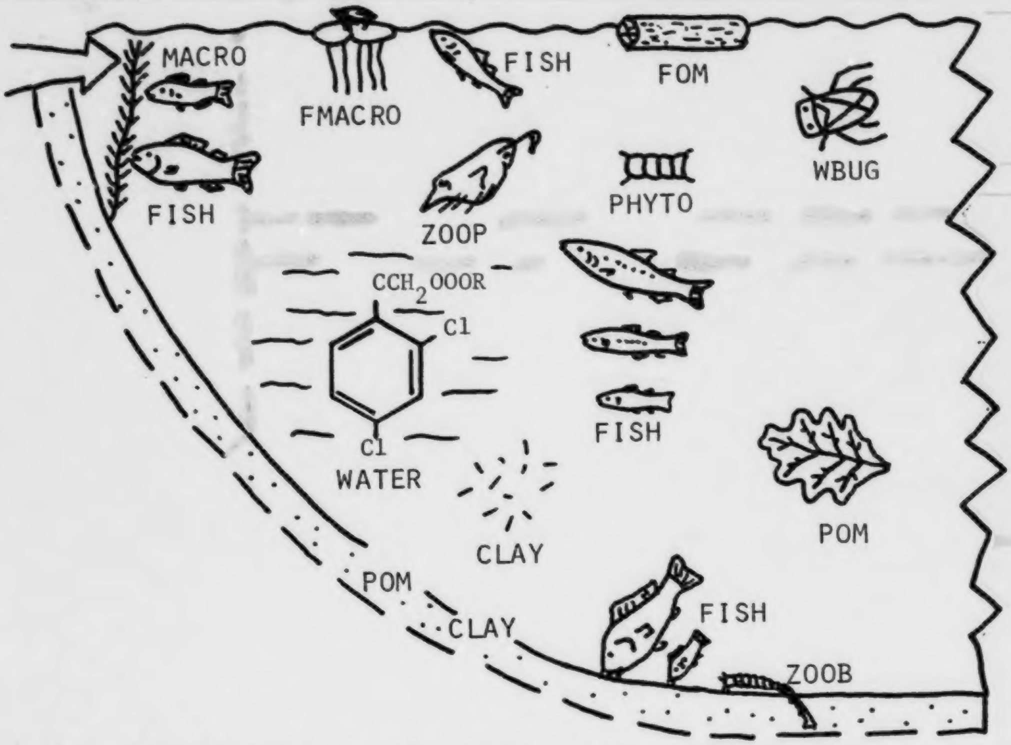

Figure 1. Compartments in the PEST model. FMACRO = floating macrophyte, MACRO = macrophyte, FOM = floating organic matter, POM = particulate organic matter, WBUG = water bug, ZOOB = zoobenthos, ZOOP = zooplankton, PHYTO = phytoplankton.

TABLE 1. STATE VARIABLE EQUATIONS

ANIMALS (zooplankton, zoobenthos and/or fish)

State Variables 1-10

$$dC/dt = CONS-EX-DEF-MORT+BSORP+GILSRP-BTRANS+LOADS \quad \text{(Eq. 1)}$$

where

C = concentration of toxic organic material (TOM)
CONS = intake of TOM through consumption
EX = loss through excretion
DEF = loss through defecation
MORT = loss through mortality of carrier organisms
BSORP = intake through passive sorption onto body
GILSRP = intake through sorption onto gill as a consequence of respiratory activity

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3/8"
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BTRANS = biological transformation of TOM
LOADS = input of TOM into ecosystem segment as a result of movement of carrier organisms

PLANTS (phytoplankton and/or macrophytes)

State Variables 11 and 12

$$dC/dt = \mathrm{BSORP-BTRANS-MORT-CONS+LOADS-MMET} \qquad \text{(Eq. 2)}$$

WATER (DISSOLVED PHASE)

State Variable 13

$$dC/dt = \mathrm{-HYDR-OXID-PHOT-VOLAT+SOLU-BSORP-GILSRP-SORP+LOADS-MMET} \qquad \text{(Eq. 3)}$$

where

HYDR = loss through hydrolysis
OXID = loss through oxidation
PHOT = loss through photolysis
MMET = loss due to microbial metabolism
VOLAT = loss through volatilization
SOLU = addition through solution
SORP = loss through sorption (or gain through desorption)

PARTICULATE ORGANIC MATTER (POM)

State Variable 14

$$dC/dt = \mathrm{-HYDR-OXID+MSUM+DEF-MMET-CONS-PHOT+SORP+LOADS} \qquad \text{(Eq. 4)}$$

where

MSUM = addition of TOM due to mortality of carrier organisms

FLOATING ORGANIC MATTER (FOM)

State Variable 15

$$dC/dt = \mathrm{-VOLAT-MMET-CONS+DEF-HYDR-OXID-PHOT+SORP-SOLU+LOADS} \qquad \text{(Eq. 5)}$$

CLAY

State Variable 16

$$dC/dt = \mathrm{-MMET-CONS+DEF-HYDR-OXID-PHOT+SORP-SOLU+LOADS} \qquad \text{(Eq. 6)}$$

EPA-287 (Cin.)
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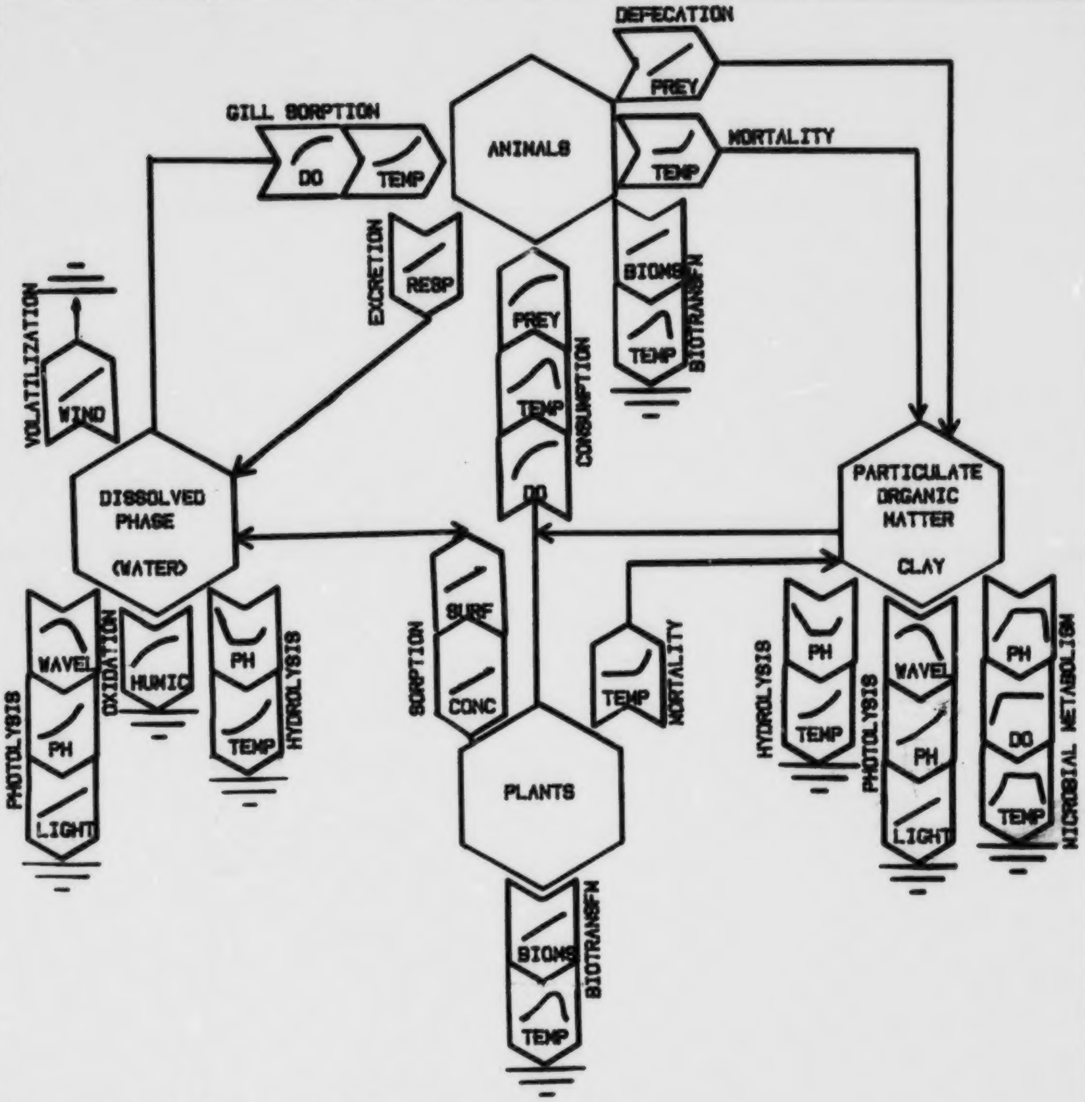
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VOLATILIZATION
WIND
DISSOLVED PHASE (WATER)
PARTICULATE ORGANIC MATTER
CLAY
WAVEL
PH
LIGHT
PHOTOLYSIS
OXIDATION
HUMIC
PH
TEMP
HYDROLYSIS
SORPTION
SURF
CONC
TEMP
MORTALITY
HYDROLYSIS
PH
TEMP
PHOTOLYSIS
WAVEL
PH
LIGHT
PH
DO
TEMP
MICROBIAL METABOLISM
PLANTS
BIOMS
TEMP
BIOTRANSFM

Figure 2. PEST process flow chart.

Output from the model includes: (1) the time-varying concentration of the toxic material in each carrier (in ppm), (2) the percent distribution of the toxic material among the carriers, and (3) the halflives of the toxic material in each carrier. One can also obtain plots of the degradation rates, both as they vary through time and as a function of environmental factors.

The model has been verified with process-level laboratory data for several compounds and with ecosystem data from fish ponds in Missouri and Israel and from a reservoir in Iowa. The

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BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

site constants and environmental driving variables for these ecosystems constitute useful "prototype" data sets that enhance the value of the model for evaluative purposes. The process-level results from our studies and from our summarization of the literature are used as examples in the following section.

SECTION 2

PROCESS EQUATIONS AND PARAMETERIZATION

HYDROLYSIS

HYDR

PEST represents the degradation of the TOM through hydrolysis as:

$$\text{HYDR} = (\text{TCORR*KO+TCORR*KH*}10^{-\text{pH}}\text{+TCORR*KOH*}10^{\text{pH}-14}$$
$$\text{+KA*HA+KB*HB+TCORR*KCAL)*CONCEN} \qquad \text{(Eq. 7)}$$

This includes the temperature correction factor for the Xth rate constant based on the standard Arrhenius energy equation:

$$\text{TCORR(X)} = \text{X*e}^{\left(\frac{\text{EN}}{1.987(\text{TEMP}+273)} - \frac{\text{EN}}{1.987(\text{TCOPT})}\right.} \qquad \text{(Eq. 8)}$$

where

e = natural exponent
EN = activation energy for effect of temperature on particular reaction (cal/mole)
TEMP = ambient temperature (°C)
TCOPT = temperature at which rate constant was obtained (°K)

with 1.987 being the universal gas constant and 273 being the conversion to °K.

The other terms in Eq. 7 are:

KO = uncatalyzed rate constant (1/days)
KH = acid-catalyzed rate constant (1/M days, where M is molality)
KOH = base-catalyzed rate constant (1/M days)
pH = ambient pH
KCAL = rate constant to account for colloidal, metal-ion, and phase-transfer catalysis adjusted for site conditions (1/days)
KA = rate constant for Bronsted acid catalysis (1/days)
HA = concentration of Bronsted acid (g/m^3)
KB = rate constant for Bronsted base catalysis (1/days)
HB = concentration of Bronsted base (g/m^3)
CONCEN = concentration of TOM (g/m^3)

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BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

Eq. 7 assumes that the activity of the hydrogen ion in natural waters is identical to the concentration. That is, the activity coefficient of the hydrogen ion is taken as 1. This assumption is good for natural waters containing few dissolved electrolytes (0 to 220 ppm), but will not apply in brackish or salt waters, where the total electrolyte concentration can exceed 35,000 ppm. The effect of electrolyte concentration, may be important (Walker 1976, 1978), although studies conducted in support of this project show that it has little effect on the hydrolysis of some compounds such as atrazine (Herbrandson, et al., 1977).

The uncatalyzed, acid-catalyzed, and base-catalyzed rate constants chosen for these equations are the specific rate constants that measure the contribution to the disappearance rate due to specific types of catalysis. These are easy to measure in the laboratory; determination of their values does not require detailed knowledge of the reaction mechanism. The kinetic data, however, may not fit for some compounds, and general rate constants and another rate expression may be required.

The definition of hydrolysis as the disappearance of the TOM through reaction with water does not imply a specific mechanism, and generally includes several chemical processes. Eq. 7 does assume that the rates can be expressed in terms of pseudo first-order constants, meaning that the second-order rate is made pH-dependent. By combining these constants, as in Eq. 7, the overall rate expression can model several different types of hydrogen-ion and Bronsted acid-base dependences. For example, hydrolysis rates for atrazine, malathion, carbaryl and methoxychlor can all be expressed in terms of these constants, even though atrazine reacts due to nucleophilic substitution of the hydroxide ion for the chloride ion, malathion decomposes in water due to elimination and carboxylate ester hydrolysis, carbaryl hydrolyzes by an elimination reaction, methoxychlor undergoes base-catalyzed elimination of HCL.

The pH-dependence and importance of the hydrolysis reaction vary greatly for different compounds. These variations are expressed by the relative magnitudes of the KH, KO, and KOH parameters (Table 2). Parathion is base-catalyzed (Figure 3a), pentachlorophenol is slightly acid-catalyzed (Figure 3b), methoxychlor is primarily base-catalyzed (Figure 3c), and 2,4-D is both acid- and base-catalyzed with the minimum at a pH of about 4.7 (Figure 3d).

The value for KO serves as the minimum rate of hydrolysis over the entire pH range. This is the rate constant at neutrality, where the acid and base concentrations are equal. Because the overall hydrolysis rate is the sum of the neutral, basic, acidic and miscellaneous terms, it is important when choosing hydrolysis parameters to note the overlap of KO into both acidic

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TABLE 2. PARAMETERS (1/M day) FOR SELECTED COMPOUNDS

	KH	KO	KOH	References
Methoxychlor	1.9E-3	2.57E-3	31.10	Wolfe et al., 1977 Mabey & Mill, 1978
Parathion	1.28E2	3.64E-3	2.46E3	Ketelaar & Gersmann, 1958
Pentachlorophenol	1.13E4	5.83E-3	3.34	Akisada, 1964
2,4-D	4.9E6	0	2.61E6	Wolfe et al., 1977a Zepp et al., 1975

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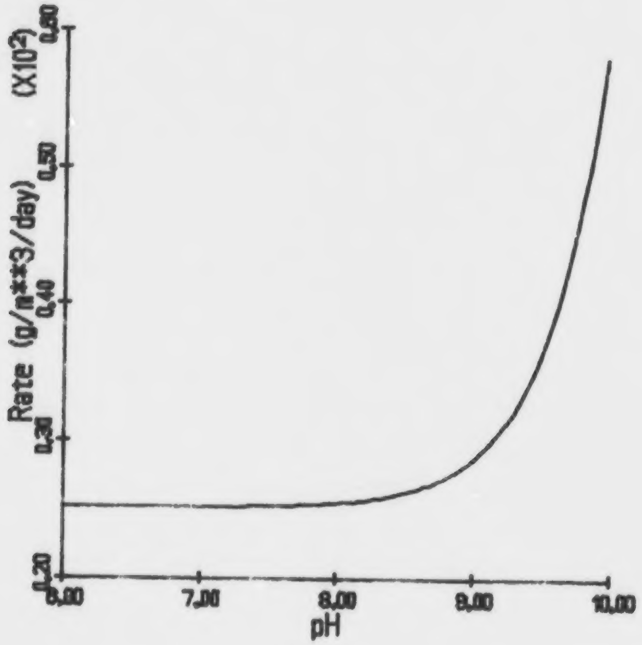

Figure 3a. Hydrolysis of parathion.

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3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

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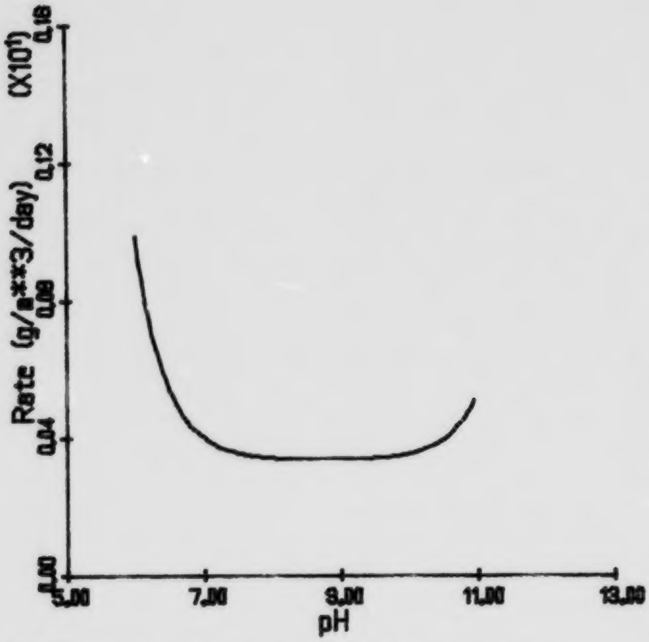

Figure 3b. Hydrolysis of pentachlorophenol.

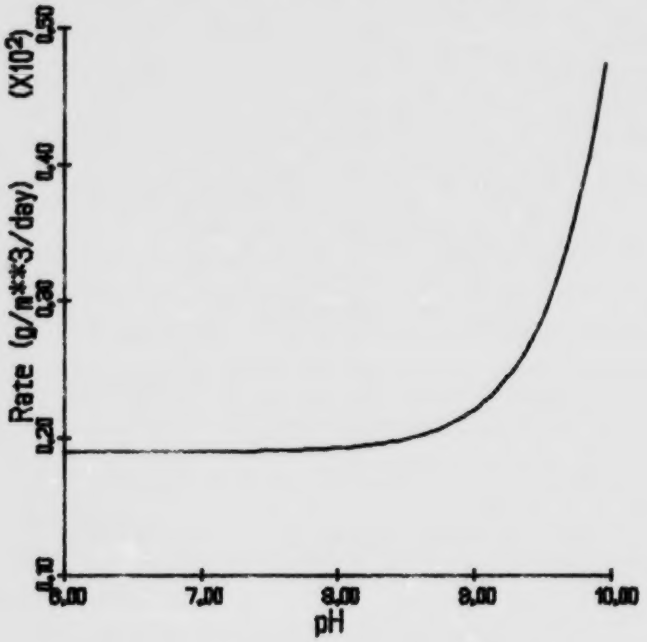

Figure 3c. Hydrolysis of methoxychlor.

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3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

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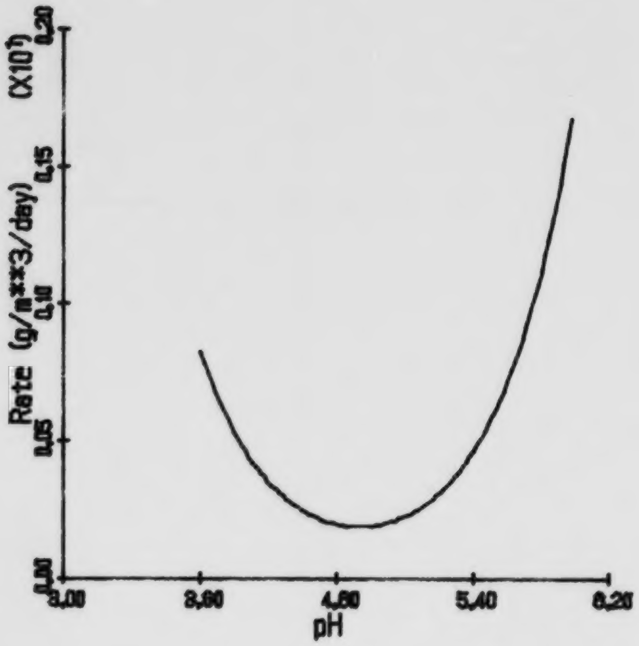

Figure 3d. Hydrolysis of 2,4-D.

and basic waters. If the overall rate constant (second order) is .001 at pH=8, then a value of KO greater than this will overshadow any KOH calculation at that pH.

For example: if a study shows that the overall hydrolysis rate of a compound is 0.1 at pH=8 and .001 at pH=7, then KO=.001 and KOH=$0.1/10^{-6}=10^{-5}$. However, if the rate at pH=8 is .0001, then KO cannot be .001. In this case the user has the choice of selecting a negative KOH and keeping KO=.001, or making up for the rate at pH=7 by choosing a large value for KH (this would be the case if there were a high degree of acid catalysis).

In this way the three rate constants are interdependent, especially around the transitions between acid and base catalysis. Because most natural waters are between pH=6 and pH=9, this range should be considered when choosing parameters. It may be necessary to sacrifice accuracy at extreme pH's in order to gain a more accurate model over this middle range.

Each of the pseudo first-order rate constants is easily obtained by dividing the rate at a given pH by the ion concentration, giving units of g/m^3 day M. In general there are two forms in which hydrolysis parameters are available. The first

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

is in the form of either first- or second-order rate constants. These can be used (after conversion to pseudo first-order constants) without considering the effects at transition regions of pH. Secondly, the parameters can be obtained from half-life values; however, care must be taken when calculating rate constants not to allow an overlap of rates which would give inaccurate results. The best way to do this is to find KOH and KH at pH's far enough away from neutrality that there is no interference. Also, if there is a high degree of catalysis, either acidic or basic, then there will be little effect of the KO value at a more extreme pH.

KA and KB add the effects of Bronsted type acids and bases to those of the hydronium and hydroxide ions. Again, the magnitude of these terms will vary with the TOM and the acids or bases responsible for the catalysis. For example, Wolfe et. al. (1976) demonstrated that the degradation of malathion is not subject to general base catalysis. If the presence of acids and bases other than hydronium and hydroxide ions is suspected in natural waters, then experimentally determined rate constants must be included as parameters in the model. Exclusion of such data may eliminate a significant portion of the total rate for hydrolysis (and provide a "worst case" simulation).

The empirical term KCAL in the rate expression accounts for catalysis by suspended colloidal materials, sediment organic matter, metal ions, phase transfer catalysis, and any other factors which increase or decrease the rate of TOM hydrolysis. Such effects may make a significant contribution to the total hydrolysis rate. For example, Li and Felback (1972) demonstrated that the presence of humic acids increases the rate of atrazine hydrolysis 50-fold. Khan (1978) observed increased hydrolysis rates for atrazine in water containing fulvic acids. Herbrandson et al. (1977) as a part of this project have shown that colloidal catalysis is highly dependent on the chemical nature of the colloids, and can vary, in the case of atrazine, from significant acceleration to no effect at all. Armstrong et al. (1967, 1968) concluded that sterile soil particles increase the rate of atrazine hydrolysis almost 10-fold, while White (1976) found evidence of the hydrolysis of many S-triazines on the acidic surface of montmorillonite. On the other hand Skipper (1978) found no S-triazine hydrolysis in allophanic clay colloids. Harris (1967) correlated the rate of hydrolysis of simazine VIII (a chloro-S-triazine) with the percent oxidizable carbon present in the soil.

Metal ions can accelerate, decelerate or have no effect on pesticide hydrolysis rates in both aqueous solution and on the surface of colloidal clays. Copper (II) ions accelerate hydrolysis of Dursban, Diazinon, Ronnel, and Zytron (organic phosphorus pesticides structurally similar to malathion) at 20°C. Acceleration is proportional to the ratio of copper ion

EPA-287 (Cin.)
(4-76)

concentration to pesticide concentration. The rate increases as this ratio increases until equal concentrations are present, after which the rate stays constant. Co^{++}(aq), Zn^{++}(aq), Ni^{++}(aq), and Ca^{++}(aq) do not catalyze the hydrolysis of these compounds, however. First-order kinetics are observed for both the accelerated and uncatalyzed reactions, except in the case of Dursban, which reacts at a rate proportional to the square of the Dursban concentration (Mortland and Raman, 1967). Similarly, Ketelaar et al. (1956) observed a 20-fold rate increase in parathion hydrolysis when both metal ion and pesticide are present in milli-molar quantities. He found only doubling of the rate for paraoxon present. First-order kinetic behavior is found in both of these cases. Copper ions bound to soil organic material do not catalyze the hydrolysis of organic phosphorus pesticides (Mortland and Raman, 1967). These observations, and the low, naturally occurring concentrations of Cu^{++}(ag) (1.2 to 53 ppb) (Wetzel, 1975) have led at least one group to discount metal-ion catalysis as being important in environmental systems (Mabey and Mill, 1978). More research in this area is needed, however, before this effect can be ignored or included in fate modeling.

KCAL has been included in Eq. 7 to adjust the overall rate for these effects because no comprehensive theoretical expression for the rate constant due to these effects has been proposed, and because the magnitude of these effects vary with site composition and TOM concentration. This term may be determined empirically by measuring the rate of hydrolysis in natural waters, then subtracting the known rate constants from the overall rate constant. Alternatively, it can be estimated from data in the literature for the types of phenomena just discussed. Eventually, however, catalysis from these other sources will have to be demonstrated and quantified if the model is to yield accurate predictions.

Because the pH-dependence of hydrolysis can cause orders-of-magnitude differences in degradation rates within the range of pH found in natural aquatic environments, it is necessary to pay close attention to the pH loadings used in a particular simulation. The pH in an unbuffered, highly-productive fish pond can vary by three units in the course of a day; this should be represented by a carefully weighted average because the present version of PEST does not simulate diurnal variations.

Verification

The results of the hydrolysis calculation for several compounds are presented in Table 3. The results are expressed in terms of half-lives and are compared with literature values under similar conditions. Without exception, the comparisons of PEST half-lives with literature values show that the hydrolysis submodel is accurate. All the values are of the same order of magnitude, and usually within 30% of the quoted literature

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TABLE 3. COMPARISON OF PEST HYDROLYSIS HALF-LIVES WITH LITERATURE VALUES FOR VARIATIONS IN pH AT CONSTANT TEMPERATURE

Pesticide	Conditions	PEST		Literature	
1) Carbaryl	pH=5	5.2	years	3.6	years
	pH=6	6.3	months	4.4	months
	pH=7	19	days	13	days
	pH=8	1.9	days	1.3	days
	pH=9	4.5	hours	3.2	hours
2) 2,4-D	pH=6	39.4	days	44	days
	pH=9	.96	hours	.96	hours
3) Methoxychlor	pH=9	267	days	270	days
4) Malathion	pH=6	228	days	150	days
	pH=7	23.4	days	15.0	days
	pH=8	2.29	days	1.5	days
	pH=9	.234	days	0.15	days
6) PCP	pH=6	69	days*		
	pH=7	173	days	n.a.	
	pH=7.5	210	days		

*The slight acid catalysis shown here is a result of the photolysis observations of Akisada (1964), in which photolysis was 3 times faster under acidic conditions. Because there is no method for modeling ionic influence in the photolysis program, any catalysis will have to be accounted for in the hydrolysis calculation.

values. A brief analysis of these results follows:

Carbaryl — PEST half-life values are consistently 31% higher than the literature numbers. The pH sensitivity is very good, and the fact that the difference in value is 31% over the whole range shows that the acid-base relationships are reasonable. The discrepancy is due to the choice of parameters. The value chosen by Wolfe et al. (1976) for the pseudo first-order, base-catalyzed constant is 2.94 E+5, while that chosen for PEST is 4.34 E+5, based on Wolfe et al. (1978).

2,4-D (methyl ester) — Because the parameter values for 2,4-D were calculated directly from the half-life values in the literature, the results were fitted to the correct values. It is revealing to note that a perfect fit was not obtained at a pH of 6, the difference in values being about 10%. The accuracy under acidic conditions was sacrificed for accuracy in the basic range because: 1) the majority of the pH loadings for the

BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
BEGIN LAST LINE OF TEXT

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

validation site at Columbia, Missouri, are above 7.0, and 2) from the half-life values it appears that 2,4-D is base-catalyzed, and it was judged more important to have greater accuracy where half-lives are short.

Parathion — Because of the number of studies done to determine the rates of hydrolysis of parathion under various conditions, it is not surprising that the half-life values do not correlate as well as the others. The literature values quoted here were calculated from the average second-order rates compiled by Wolfe et al. (1976) while the parameters were taken from work done by Ketelaar (1950), which is included in the Wolfe compilation. The Ketelaar values were chosen because of the availability of other data in that report, including the activation energies for catalysis. Also, these half-lives were shorter and varied less with pH. The predominant form of catalysis is in the basic range, and these half lives are 15% different from the quoted literature values.

Malathion — As is the case with carbaryl, the results for malathion show the same pH relationship as their literature counterparts, but with different base values. This is again due to the parameterization.

OXIDATION OXID

Autooxidation reactions may be initiated by free radicals present at low concentrations in naturally occurring substances such as humic acids (Steellink, 1977); Schnitzer and Khan, 1972) by free radicals formed thermally, or by metal ion catalysis from peroxides. Those formed from photochemical processes are considered as a part of photolysis in PEST. The rate expression used is based on first principles:

$$\text{OXID} = \text{KP}/\text{KT}^{0.5}*\text{KEFF}*\text{RAD}^{0.5}*\text{CONCEN} \qquad \text{(Eq. 9)}$$

where

KP = the rate of the reaction between the TOM and alkoxy and peroxy radicals (1/day)
KT = the rate of the competing reaction between two radicals resulting in non-radical products (1/day)
RAD = the concentration of radical initiator present in the environment
KEFF = the rate of the radical initiation reaction
CONCEN = the concentration of TOM (g/m^3)

In the case of carbaryl, 2,4-D, malathion, and atrazine, chemical oxidation contributes little or nothing to the disappearance rate (Wolfe et al., 1976). This may be due to the

EPA-287 (Cin.)
(4-76)

presence of naturally occurring, chain-terminating compounds such as amines and phenols, very low rates of initiator generation, or unreactivity of the TOM towards singlet oxygen.

Methoxychlor, on the other hand, reacts with oxygen if hydrogen peroxide is present in catalytic quantities (Wolfe, et. al., 1976). Mabey and Mill (1978), however, have estimated that the propagation step in a peroxy-radical reaction scheme would be so slow at concentrations expected in the environment that oxidation of most organics would not occur by this process.

Chemical oxidation was not modeled as a part of the verification of PEST. Oxidation of a given TOM will have to be demonstrated for the site waters being modeled if this term is to be included. The rate constants KT, KP, and KEFF will, in any case, be empirically determined.

PHOTOLYSIS

PHOT

The degradation of the TOM due to interaction with light includes both direct and sensitized photolytic reactions. Direct photolysis is treated mechanistically by PEST whereas sensitized photolysis is treated empirically. The formulation is:

$$\mathrm{PHOT} = (\mathrm{PSIA}*\mathrm{KA}+\mathrm{PSIB}*\mathrm{KSEN})*\mathrm{CONCEN}(\mathrm{I}) \qquad \text{(Eq. 10)}$$

where

KA = the sum of the wavelength-specific, direct photolysis rate constants (1/day)
PSIA = the direct photolysis quantum yield for the TOM (unitless)
PSIB = the sensitized photolysis quantum yield for the TOM (unitless)
KSEN = the rate constant for sensitized photolysis, determined empirically (1/day)
CONCEN(I) = the concentration of the TOM (g/m^3)

The first term in Eq. 10 accounts for direct photolysis and is based on the work of Zepp and Cline (1976). Rates are computed for each of twelve ultraviolet wavelengths (297.5, 300.0, 302.5, 305.0, 307.5, 310.0, 312.5, 315.0, 317.5, 323.1, and 330.0 nanometers):

$$\mathrm{KA} = \mathrm{KLAM}(297.5)+\mathrm{KLAM}(300.0)+\ldots\mathrm{KLAM}(330.0) \qquad \text{(Eq. 10a)}$$

$$\mathrm{KLAM}(\mathrm{I}) = \mathrm{IILAM}(\mathrm{I})*\mathrm{ELAM}(\mathrm{I})*\mathrm{INT}/(6.02\mathrm{E}20*\mathrm{ALPHA}(\mathrm{I})) \qquad \text{(Eq. 10b)}$$

$$\mathrm{IILAM}(\mathrm{I}) = (\mathrm{IDLAM}(\mathrm{I})*(1-10**(-\mathrm{ALPHA}(\mathrm{I})*\mathrm{LD}))+\mathrm{ISLAM}(\mathrm{I})*(1-10**(-\mathrm{ALPHA}(\mathrm{I})*\mathrm{LS})))/\mathrm{D} \qquad \text{(Eq. 10c)}$$

EPA-287 (Cin.)
(4-76)

LD = D*1.14

LS = D*1.2

IDLAM(I) = INTENS(I)*FRACD(I) (Eq. 10d)

ISLAM(I) = INTENS(I)*FRACS(I) (Eq. 10e)

INTENS(I) = INTEN*LAM(I)

where

ELAM(I) = molar extinction coefficient for the compound at the Ith wavelength (l/mole cm)
INT = the width of the wavelength interval on which the designated wavelengths are centered (nm)
ALPHA(I) = extinction coefficient for site waters at Ith wavelength (l/cm)
D = median depth of water (cm)

FRACD(I) = fraction of irradiance that is direct at Ith wavelength (supplied in program) (unitless)
FRACS(I) = fraction of irradiance that is indirect (sky) (supplied in program) (unitless)

LD and LS = effective direct and diffuse underwater path lengths for irradiance assuming a refractive index of 1.34 and solar inclination of 40° (cf. Zepp and Cline, 1977)
LAM = wavelength (nm)

There are several constants in the formulation. 6.02E20 is a factor to convert from photons to mole of photons (photons l/Einstein cm^3). 1.14 is the secant of the refracted angle of light and 1.2 is the correction for the refraction of diffuse light.

ELAM and PSIA represent the molar extinction coefficients at the twelve wavelengths, and the direct photolysis quantum yield. There have been many studies to determine quantum yields, and most extinction coefficients are available from spectroscopy references (such as the Sadtler series). It is important to note the solvent used for the extinction measurement, as a non-organic solvent is preferred.

The difference between the approach used in PEST and that of Zepp and Cline (1977) is that PEST uses loadings rather than calculating solar intensity as a function of latitude and season. The values for solar intensity are entered as weekly values of Langleys/day, the most common unit of solar irradiance; these data are available for all U.S. Weather Bureau stations.

EPA-287 (Cin.)
(4-76)

The intensity at each wavelength is determined by multiplication of the intensity loading by the arrays FRACS and FRACD. These two twelve-unit arrays represent the fraction of direct and sky (diffuse) radiation at the wavelengths considered. These have been calculated from data published by Green (1976), and Bener (1972), and compare reasonably well with the results of the Zepp and Cline (1977) model (Table 4).

TABLE 4. COMPARISON OF THE SOLAR INTENSITY BREAKDOWN IN PEST WITH THE RESULTS OBTAINED BY ZEPP AND CLINE (1977)

Wavelength	Direct	Diffuse	Total	W (Zepp & Cline)
297.5	.3033 E 12	.5035 E 12	.8067 E 12	.648 E 12
300	.9590 E 12	.2309 E 13	.3268 E 13	.219 E 13
302.5	.3291 E 13	.4997 E 13	.8288 E 13	.657 E 13
305	.1188 E 14	.1544 E 14	.2732 E 14	.163 E 14
307.5	.1243 E 14	.2556 E 14	.3800 E 14	.274 E 14
310	.1707 E 14	.3706 E 14	.5413 E 14	.444 E 14
312.5	.2019 E 14	.5414 E 14	.7433 E 14	.643 E 14
315	.2412 E 14	.7488 E 14	.9900 E 14	.836 E 14
317.5	.2814 E 14	.1027 E 15	.1309 E 15	.103 E 15
320	.6881 E 14	.1122 E 15	.1810 E 15	.121 E 15
323.1	.1467 E 15	.1571 E 15	.3038 E 15	.226 E 15
330	.4038 E 15	.4521 E 15	.8559 E 15	.762 E 15

Assumptions:
1) Midsummer sun (approximately 550 ly/day) at 40° north latitude
2) Atmospheric Ozone content equal to .320 cm STP
3) Index of refraction of water equal to 1.34

The advantage of the loading approach used in PEST over the computation approach is that variations in total solar intensity due to cloud cover and elevation are accounted for. However the distribution over the ultraviolet range is affected by both cloud cover and ozone variations, and this is not accounted for in PEST.

The site constants for direct photolysis are the depth of the section being studied and the attenuation of the site water. The depth (D) is the median depth of the water and has units of centimeters. The twelve-member array ALPHA represents the attenuation coefficients of the site water, and has units of inverse centimeters. These coefficients are an important set of parameters for the photolysis calculation, and the overall rate of photolysis can vary 50-fold over the reported range of values.

EPA-287 (Cin.)
(4-76)

If no precise values for attenuation are available for the site studied, it is helpful to have at least a qualitative description of the clarity of the water, so that an educated guess can be made as to which set of coefficients will be used. Two sets of coefficients are listed in Table 5, the first for pure water (Hautala, 1978) and the second for a sampling of southern river waters (Zepp and Cline, 1977). For most applications a scaled-up set of coefficients could be derived. The values for river water should serve only as an upper limit, as these are taken from waters that are highly colored, and may be as much as 95%different (by admission of the authors). If a set of coefficients is estimated based on qualitative observations (or Secchi disk measurements) it is important that the relative values at the twelve wavelengths be similar to those listed in Table 5. Thus the attenuation in the UV region will decrease with increasing wavelength, and will approximately double from 297.5 to 330 nanometers. Table 6 presents the results of a sensitivity analysis which is helpful in judging the effect of increased attenuation on the photolysis half-life.

TABLE 5. ATTENUATION COEFFICIENTS (AS PRESENTED BY HAUTALA, 1978, AND ZEPP AND CLINE, 1977).

Wavelength	Pure Water	River Water
297.5	.0028	.123
300.0	.0028	.121
302.5	.0026	.119
305.0	.0025	.117
307.5	.0024	.116
310.0	.0023	.114
312.5	.0022	.112
315.0	.0021	.111
317.5	.0020	.109
320.0	.0019	.107
323.1	.0018	.105
330.0	.0015	.100

The direct photolysis rate expression, as written, does not include the effect of hydrogen ion concentration. If this effect has been shown to be important, as it has for 2,4-D (Aly and Faust, 1964), and 2,4,5-T(I) (Crosby and Wong, 1973), then allowance must be made by changing the form of the equation appropriately. For example, if it can be shown that the reactionate for 2,4-D is proportional to the equilibrium concentration of the 2,4-D-Chloropheroxyacelate anion (2,4-DOO-) (II),

EPA-287 (Cin.)
(4-76)

TABLE 6. ATTENUATION SENSITIVITY ANALYSIS OF PENTACHLOROPHENOL UNDER MIDSUMMER SUN

ALPHA	Half-life for Photolysis	Percent reduction from ALPHA=.0025
.0025	00.539 days	---
.0050	00.746	38%
.0100	01.25	132%
.0250	02.99	455%
.0500	05.98	1010%
.1000	11.96	2119%

the concentration of which is itself proportional to the hydrogen ion concentration, then KA might be rewritten as

$$KA = (KIAM_{297.5}+KIAM_{300.0}+\ldots KLAM_{330.0}) *KEQ/10^{-pH} \qquad \text{(Eq. 10b)}$$

where KEQ is the equilibrium dissociation constant at the site temperature.

$$KEQ = KA = (H^{+}(aq))(2,4\text{-}DOO)/-/(2,4\text{-}D) \qquad \text{(Eq. 10c)}$$

The molar extinction coefficients used for each wavelength would then be those associated with the anion. The rest of Eq. 10 remains the same in this case.

Sensitized photolysis is calculated using an empirically determined, site-specific rate constant; this should be modified at the user's discretion to reflect the observed kinetic behavior of the target compound.

The relationship between KSENS and the incident direct and sky light intensity also must be empirically determined. The simplest model assumes a linear relationship where

$$KSEN = KMEAS*IITOT/IIMEAS \qquad \text{(Eq. 10d)}$$

where

$$IITOT = IILAM_{297.5}+IILAM_{300.0}+\ldots IILAM_{330.0}$$

IIMEAS is the light intensity integrated over the same wavelengths and time period as IILAM.

LSM, LDM are experimentally measured effective path lengths for light in the reactor, IDMLAM, ISMLAM are the measured direct

EPA-287 (Cin.)
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and diffuse light intensities at a particular wavelength in the reactor, and ALPHA is the absorption coefficient of the water used in the reactor at a particular wavelength. Most literature gives the total incident power and some impression of the wavelength distribution in the reactor. To a rough approximation, then, if the reaction vessel is not too large, if distilled water is used in the medium, and if the wavelength interval of the irradiating list is about 295nm to 330nm, the reported incident power IIMEAS can be used after it is converted to approximate units (photons/cm^2). Better equations exist in the literature; see, for example, Boval and Smith (1973).

Very few quantitative data are available in the literature on the kinetics of sensitized photolysis in natural waters. The parameters are usually determined by back-calculation from an observed half-life value. There are few studies that provide the experimental data necessary to fit the required parameters. Most studies provide only a half-life observation under certain solar conditions (e.g., midsummer). The routine sums up the energy absorbed at each wavelength, and uses this sum as the driving force for the sensitized mechanism. The total energy is multiplied by the sensitized rate constant (KMEAS), and is divided by the energy for which the rate was determined. In this way the rate at a given energy is corrected for the energy of the site.

In determining values for KMEAS for half-life measurements, a trial and error method is used. It is helpful to have a self-contained version of PHOT so that values for KSENS'(the overall sensitized rate) can be read directly and compared with the reference half-life. The sensitized quantum yield (PSIB) may be assumed equal to the direct quantum yield if no other information is available. IIMEAS, the experimental energy value, may be set to a standard 3 E13 (photon/cm^2s). At this point KMEAS can be varied until the half-lives obtained compare favorably with the reference values.

Verification

The results of the photolysis calculations for several compounds are compared with the literature values in Table 7. It should be noted that the sensitized half-lives for both Methoxychlor and Malathion are much longer than the literature values quoted. This is because the literature values are taken from experiments done in river water, which contains higher amounts of colored and other material which may serve as sensitizing agents. The desired rates in lake water were judged to be lower, and so smaller values for KMEAS were chosen.

The relationship of photolysis to solar intensity and the effect of sensitized photolysis are illustrated by Figures 4a, 4b, and 4c.

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(4-76)

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TABLE 7. COMPARISON OF PEST PHOTOLYSIS HALF-LIVES WITH LITERATURE VALUES

The range of PEST half-lives corresponds to a range of intensity from 400 to 600 ly/day. This corresponds to the season from midspring to midsummer. The conditions column refers to the season in which the literature value was taken.

Pesticide	Condition	Literature	PEST
Carbaryl	midsummer	2.14 days	1.66 - 2.48 days
Atrazine	artificial	1.04 days	.723 - 1.08 days
Methoxychlor (sensitized)	midsummer	2-5 hours	8.4 - 12.5 hours
(unsensitized)	midsummer	4.5 months	2.13 - 3.18 years
Parathion	midsummer	6.81 days	9.93 - 14.8 days
Malathion (sensitized)	September	15 hours	11.2 - 16.8 days
(unsensitized)		*	5.5 - 8.2 months
Pentachlorophenol		†	0.86 - 1.28 days
2,4-D	September	29 days	28.9 - 43.3 days

*Malathion photolysis is described as the slowest of any pesticide studied under non-sensitized conditions by Wolfe et al. (1976). However, unlike methoxychlor sensitization, malathion sensitization has only been observed in one water sample. Therefore it is recommended that malathion photolysis be considered only as a direct mechanism.

†Photolysis of pentachlorophenol was described by Crosby (1972) as being complete in 5 to 7 days in natural waters. Taking five half-lives as the length of time for 95 percent degradation, total degradation would take 4.3 to 9.4 days as calculated by PEST.

As with hydrolysis, photolysis proceeds at different rates for different compounds and in different chemical environments. Direct photolysis is probably not as important as hydrolysis for atrazine, methoxychlor, malathion, or 2,4-D, but may be the rate-controlling process for carbaryl degradation. Sensitized photolysis is very rapid, however, for methoxychlor and malathion in natural river waters (Wolfe et al., 1976).

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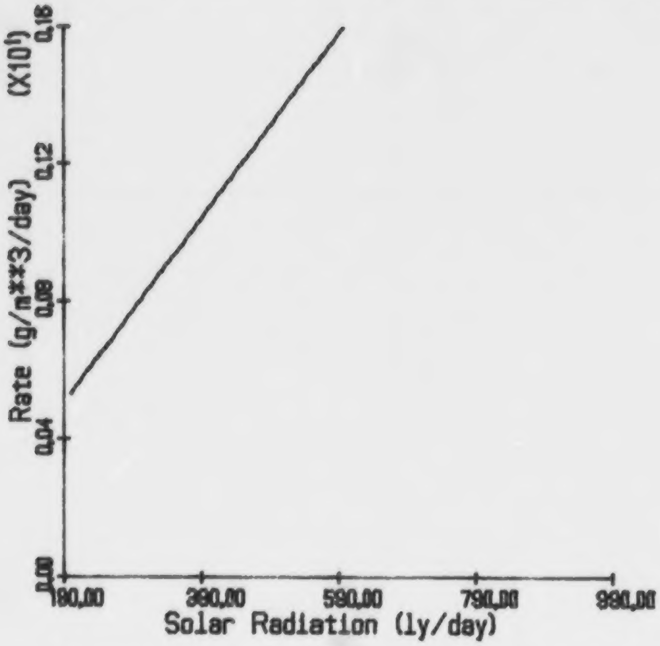

Figure 4a. Sensitized photolysis of methoxychlor.

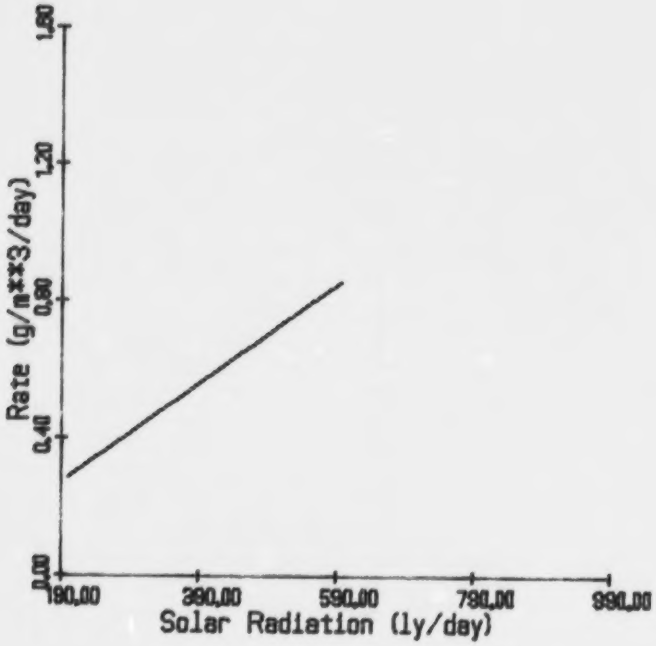

Figure 4b. Unsensitized photolysis of methoxychlor.

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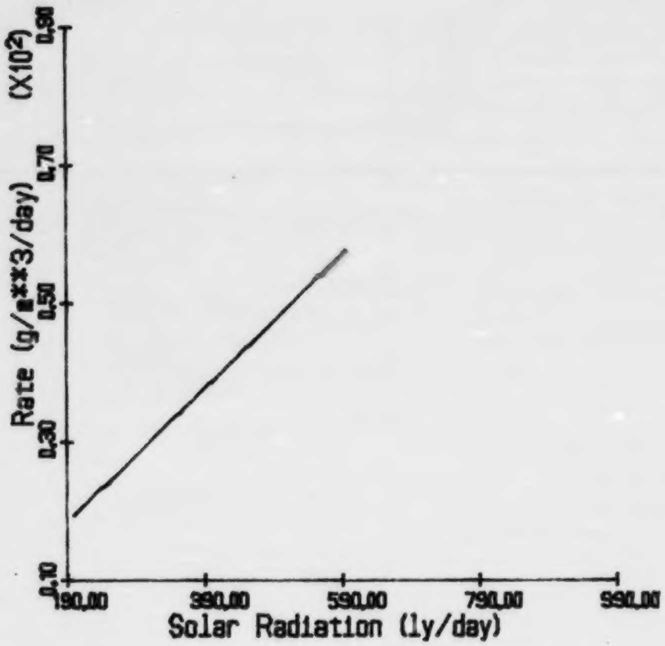

Figure 4C. Photolysis of Pentachlorophenol.

VOLATILIZATION VOLAT

The rate at which a toxic organic material (TOM) will volatize can be expressed as:

$$\text{VOLAT} = \text{CONCEN}*\text{KLEXPT}/(1/\text{KLIQ} + 1/\text{KGAS}) \qquad \text{(Eq. 11)}$$

where

VOLAT = mass transfer rate (moles/cm^2/hr)
CONCEN = concentration (moles/cm^3)
KLEXPT = correction factor, where experimental data are available, otherwise = 1 (unitless)
KLIQ = liquid-phase mass transfer coefficient (cm/hr)
KGAS = gas-phase mass transfer coefficient (cm/hr)

The denominator is the sum of the liquid- and gas-phase mass transfer resistances.

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

Because of the difficulty in measuring interfacial conditions, it is convenient to express the transfer rate in terms of an overall driving force and the total resistance, made up of the individual resistances in the gas and liquid films. This treatment is directly analogous to that used in treating convective heat transfer using the Whitman two-film theory (Whitman, 1923).

This approach considers the existence of a gas film and a liquid film forming an equilibrium interface. Within the films transfer is by diffusion, providing a resistance to flow. The thickness of the films, and consequently the resistance, is considered to be a function of the nature of the fluid and the turbulence within the fluid. This concept is illustrated by Figure 5.

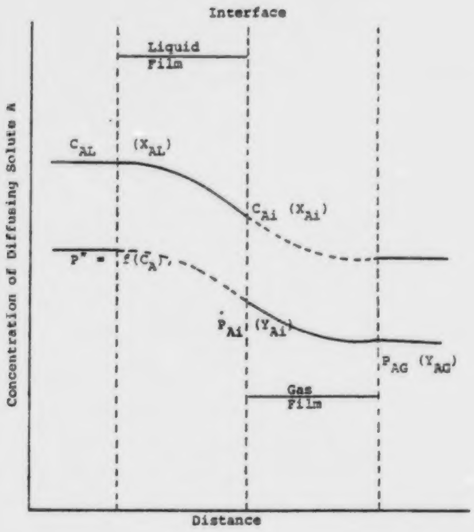

Figure 5. Two-film model of volatilization from the surface of water (from Sharma, 1979).

The concept of such discontinuities is perhaps physically unrealistic. However, the approach has proven useful as an aid for visualizing processes at the interface and for simplifying theoretical calculations of exchange rates. In this application, we are concerned with a TOM dissolved in water and diffusing into the air. The TOM will encounter resistance to transfer through the water immediately adjacent to the interface between the water and the air. This is the liquid film. The TOM must then diffuse through a gaseous film where it again encounters resistance to flow.

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Gas-phase Mass Transfer Coefficient KGAS

Not many values are available for gas-phase mass transfer coefficients. An empirical relationship as a function of wind is based on Liss (1973):

KGAS (water) = (0.1857+11.36*WINDV*100)/100 (Eq. 13)

where

WINDV = wind velocity (m/sec)

This coefficient can then be used to obtain the gas-phase coefficient for the TOM, corrected for the diffusion coefficient ratio (Othmer and Thakar, 1953; cf. p. 29 this report):

KGAS = KGAS(water)*HENRY*(VH20/VTOM)**0.6/ ((TEMP+273.15)*8.206*10**-7) (Eq. 14)

where

HENRY = Henry's Law Constant (atm·cm^3/mol)
VH20 = molal volume of water (cm^3/mol)
VTOM = molal volume of TOM (cm^3/mol)
TEMP = ambient temperature (^oC)

The 8.206*10**-7 factor is the gas constant (cm^3.atm/mol K) and 273.15 is used to convert ^oC to ^oK. Henry's Law constant may be calculated as:

HENRY = VPRESS*MOLCWT/(760*SOLUB) (Eq. 15)

where:

MOLCWT = molecular weight (unitless)
SOLUB = solubility (mol/cm^3)
VPRESS = vapor pressure (atm)

Table 8 lists values for several compounds calculated using this procedure. The molecular volume VTOM can be calculated as the sum of the contributions of each element in the compound. Table 9 lists the contributions of common elements and structural configurations (Perry, 1963). Calculated values are given for water, benzene, and selected pesticides in Table 10.

It has been shown that environmental values of KGAS and KLIQ are such that KGAS/KLIQ normally lies in the range of 50 to 250 (Sutherland, 1978). In addition, it may be noted that for values of HENRY below 5 E-6 (corresponding to relatively high

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

TABLE 8. CALCULATED HENRY'S LAW CONSTANTS

Compound	HENRY
Atrazine	2.58 E-9
Carbaryl	1.32 E-6
Dieldrin	5.40 E-5
Malthion	3.74 E-7
Methoxychlor	1.00 E-5
Parathion	6.06 E-7
Pentachlorophenol	3.10 E-6
2,4-D	3.15 E-8

TABLE 9. LE BAS ADDITIVE VOLUMES TO CALCULATE LIQUID MOLAL VOLUME (cc/g mole)

Atomic Volumes:

As	30.5	F	8.7	P	27.0	Sn	42.3
Bi	48.0	Ge	34.5	Pb	48.3	Ti	35.7
Br	27.0	H	3.7	S	25.6	V	32.0
C	14.8	Hg	19.0	Sb	34.2	Zn	20.4
Cr	27.4	I	37.0	Si	32.0		

Chlorine -	
Terminal (as in R-Cl)	21.6
Medial (as in R-CHCL-R)	24.6
Nitrogen -	
Double bonded	15.6
Triple bonded	16.2
In primary amines (R-NH2)	10.5
Secondary amines (R-NH-R)	12.0
Tertiary amines (R3-N)	10.8
Oxygen - 7.4 (except as noted below)	
In methyl ester	9.1
In methyl ethers	9.9
In higher esters, ethers	11.0
In acids	12.0
In union with S,P.N	8.3
Deductions -	
Three member ring	- 6.0
Four member ring	- 8.5
Five member ring	-11.5
Six member ring (benzene)	-15.0
Naphthalene ring	-30.0
Anthracene ring	-47.5

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EPA-287 (Cin.)
(4-76)

TABLE 10. CALCULATED OR OBSERVED MOLAL VOLUMES FOR SELECTED COMPOUNDS

Compound	Molal Volume
Dissolved Oxygen	14.8
Water	18.7
Benzene	96.0
Atrazine	229.3
Carbaryl	218.7
2,4-D	239.6
Dieldrin	314.2
Malathion	345.7
Methoxychlor	345.3
Parathion	302.6
Pentachlorophenol	192.9
Simazine	207.1

solubility or low vapor pressure) the transfer is gas-phase controlled. On the other hand, for values above 5 E-3 the liquid phase controls.

Liquid-phase Mass Transfer Coefficient

The computation of the liquid-phase mass transfer coefficient (KLIQ) involves two equations according to wind velocity. For velocities below 3 m/sec, where calm water prevails, an empirical, linear equation is used:

```
KLIQ = ((WINDV*100*1.287)/300+2.5)*1.016**
       (TEMP-20)*(VBEN/VTOM)**0.6                    (Eq. 16)
```

where

VBEN = molal volume of benzene (cm^3/mol)

The temperature correction factor (second line of the equation) is based on the reaeration studies of Streeter et al. (1936) and was verified as a part of this study (Sharma, 1979). The fit is quite good for benzene, but only the trend is shown for toluene (Table 11).

The third factor corrects for the relative rates of the TOM and benzene. Benzene is used as a standard in PEST because 1) experimental data are available for various wind velocities, 2) it is a much larger molecule than oxygen (the other standard used in volatilization studies), and 3) it has a ring structure similar to that of many TOMs.

TABLE 11. VERIFICATION OF TEMPERATURE CORRECTION

Compound	Temperature (°C)	KLIQ Observed	KLIQ Predicted
Benzene	20	2.9	2.9
Benzene	25	3.14	3.13
Benzene	30	3.4	3.39
Toluene	20	2.91	2.91
Toluene	25	2.92	3.15
Toluene	30	3.18	3.41

(20° is reference temperature)

In a liquid with a dilute concentration of pollutant KLIQ is proportional to the diffusivity of the pollutant. Othmer and Thakar (1953) found that the diffusion coefficient in dilute aequeous solutions is inversely proportionate to the 0.6 power of the molal volume. Therefore, the transformation factor to permit the benzene data to be used is:

$$(VBEN/VTOM)^{0.6}$$

Table 12 gives experimental results obtained in this study and used to calibrate the model (Sharma, 1979).

TABLE 12. LIQUID-PHASE MASS TRANSFER COEFFICIENTS AT 25°C

Compound	Temperature	KLIQ
Benzene	25	2.90
Toluene	25	2.92
Atrazine	25	7.09×10^{-2}
Methoxychlor	25	2.29×10^{-2}
Carbaryl	25	2.01×10^{-2}

At wind velocities above 3 m/sec there is turbulent flow with waves; under these conditions Eq. 16 becomes:

$$KLIQ = (11.4*RE^{0.195}-4.1)*1.016^{(TEMP-20)}* (VBEN/VTOM)^{0.6} \qquad \text{(Eq. 17)}$$

The first factor is based on experiments by Cohen, Cocchio and MacKay (1978) using benzene that showed that:

$$KLIQ = 11.4*RE^{0.195}-4.1 \qquad \text{(Eq. 17a)}$$

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with turbulence or "roughness" represented by the dimensionless Reynolds Number (RE):

$$RE = (WINDV*100)0.17 \qquad \text{(Eq. 17b)}$$

where 0.17 is the kinematic viscosity of air (Sabersky et al., and Acosta (1964).

The other two factors correct for temperature and the relative diffusivities of Benzene and the TOM as in Eq. 16. The effect of wind is shown in Figure 6.

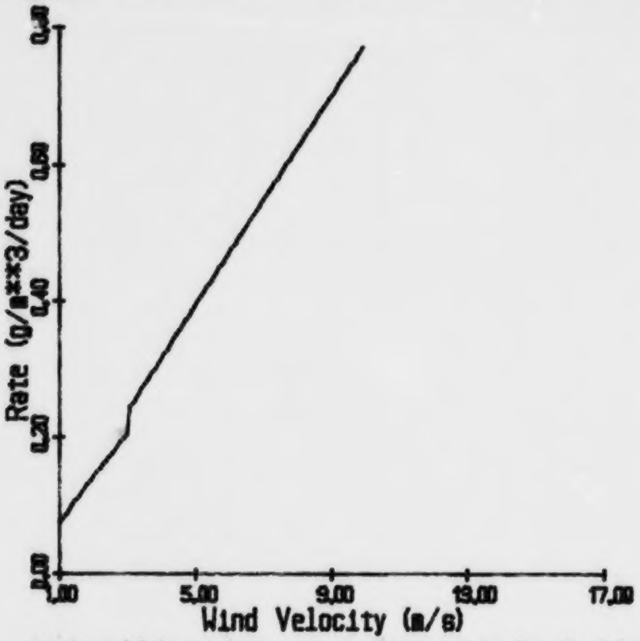

Figure 6. Volatilization of a hypothetical liquid-phase controlled compound. Note the discontinuity at 3 m/s.

Verification

The results of volatilization calculations are compared with reference values in Table 13. Although no precise values for volatilization could be found in the literature, the vaporization indices published by Haque and Freed (1975) serve as an indication of the accuracy of the submodel. For all the compounds except 2,4-D the PEST and literature ranges of values roughly coincide. For 2,4-D the only literature value available was for the acid, whereas PEST was parameterized for the methyl ester.

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

TABLE 13. COMPARISON OF PEST VOLATILIZATION RATES WITH LITERATURE VALUES

The PEST values represent the range of rates corresponding to wind velocities from 7 to 15 m/s.

Pesticide	Vaporization Index	Approximate Conversion	PEST Values
Carbaryl	3-4	1.37 - 2.74E-3	.611 - 8.53E-4
Malathion	2	.548 - 8.2E-4	.106 - 1.47E-4
Parathion	3	.959 - 1.78E-3	.118 - 1.58E-3
Atrazine	na	---	.203 - 2.83E-5
2,4-D*	1	<2.74E-5	.257 - 3.59E-3
Pentachlorophenol	na	---	.118 - 1.65E-3
Dieldrin	†	1.33E-3	2.01E-4 - 2.79E-3

[*] The literature value for 2,4-D is for the acid, while the PEST calculation is for the methyl ester.

[†] This value was calculated from a half-life value published by Mackay and Leinonen (t 1/2=1.44 years).

SOLUTION

SOLU

Solution is treated in a very straightforward manner in PEST; the formulation is intended only to keep the TOM in the dissolved phase from exceeding the solubility:

$$SOL = CONCEN(15) - EXTRA \quad \text{(Eq. 18)}$$

if $CONCEN(13)+CONCEN(15)-SOLUB*TCORR<0$: (Eq. 18a)

$$EXTRA = 0$$

otherwise:

$$EXTRA = CONCEN(13)+CONCEN(15)-SOLUB*TCORR \quad \text{(Eq. 18b)}$$

where

CONCEN(13) = concentration of TOM in water
CONCEN(15) = concentration of TOM in particulate form
TCORR = temperature correction (Eq. 8)

MICROBIAL METABOLISM MMET

The rate of microbial metabolism resulting in the degradation of TOM is computed in the subprocess routine MMET. Microbial metabolism is defined as any biochemical conversion of the parent compound by a microbial assemblage. PEST models microbial metabolism as:

$$\text{MMET} = \frac{\text{A*TADPT*METMAX*CONCEN}}{\text{KS+CONCEN}} \qquad \text{(Eq. 19)}$$

where

METMAX = chemically and photochemically corrected TOM transformation rate by an "adapted" mixed assemblage under non-limiting conditions of H^+, dissolved oxygen, temperature, nutrients and mixing (1/day)
CONCEN = concentration of TOM (g/m^3)
KS = constant equal to TOM concentration of 1/2 METMAX (g/m^3)
A = activity coefficient which reduces METMAX due to site conditions (unitless)
TADPT = effective TOM-degrading microbial biomass (g organism/m^3)

In order to model microbial metabolism of TOM, a maximum value (METMAX) must be determined which can be reduced by site correction factors (A and TADPT) as specified in the above equation.

This maximum value ideally is the rate of degradation of the chemical by a microbial assemblage with a high degree of species diversity. This assemblage should have been exposed to the compound for at least several generation times, and be growing under optimal conditions of DO, temperature, pH, nutrients and mixing. During this time some enrichment may also occur.

In order to provide for a wide range of biochemical activities, inocula from sources that are undergoing complex organic decomposition should be combined and used for the determination of METMAX (e.g. soil, marsh water, sediment). In practice, the flocculant layer of a lake sediment is well suited for these determinations by virtue of its interfacial position. Although it has a rather constant, or gradually changing, thermal environment, it is subject to random fluctuations in nutrients and dissolved oxygen as a function of mixing. As such, it is adapted to a variety of intermittent environmental conditions. This system, amended with soil and marsh inocula, can be used for TOM degradation studies. Samples obtained at peak seasonal temperatures for the system should be used because this condition would produce the most metabolically active assemblage.

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(4-76)

Values for METMAX have been derived for malathion, atrazine, and 2,4-D. The rates of degradation of these compounds were measured under anaerobic and oxygen-saturated conditions in shake flasks at 23-30°C. Sediment was taken from the littoral area of a lake (1 m depth in Lake George, New York) during the growing season (June and July). This site has a significant macrophyte cover which contributes organic matter to the underlying sediment through sloughing and death and provides for a great deal of microbial species diversity. Samples were taken of the metabolically-active surface sediments. These sediments were diluted to approximately 1 g (dry weight) per liter with lake water from the same site. The sediments were incubated with pesticide at concentrations of 50 and 100 mg/l.

The time course of TOM disappearance over a period of up to 2 weeks was followed by solvent extraction and gas chromatography using established methods. These rates were corrected for photochemical and chemical degradation with dark and inactivated systems (Hg, antibiotics, boiled). Figure 7 is an example of the efficiency of microbial metabolism under ideal conditions. In the absence of these detailed measurements of TOM disappearance, the METMAX can also be estimated from the biochemical oxygen demand (BOD) for the compound.

The need to relate biodegradation capability to the site conditions is met through the A factor. This factor modifies the maximum metabolic rate of the effective biomass (IADPT) to the rate possible under site conditions. Thus it is a reduction factor determined by the site conditions and particular TOM. The environmental factor that is most restrictive to microbial growth and decomposition of the particular TOM determines A. For example, if the TOM is aromatic and the particular compartment being modeled is the sediment during summer conditions, the limiting parameter might be DO and a correction factor based on the influence of dissolved oxygen on the metabolic rate of aromatic ring degrading organisms would be used (DOCOR) to limit METMAX.

$$A = \min(\mathrm{DOCOR}, \mathrm{PHCOR}, \mathrm{TPCOR}, \mathrm{TMIX}) \qquad \text{(Eq. 19a)}$$

where each term is a unitless reduction factor for suboptimal conditions.

The dependence of the microbial assemblage on oxygen (DOCOR) can be expressed as:

$$\mathrm{DOCOR} = \frac{\mathrm{DO2}}{\mathrm{MKO2}+\mathrm{DO2}} \qquad \text{(Eq. 19b)}$$

if DOCOR < DOMIN then DOCOR = DOMIN

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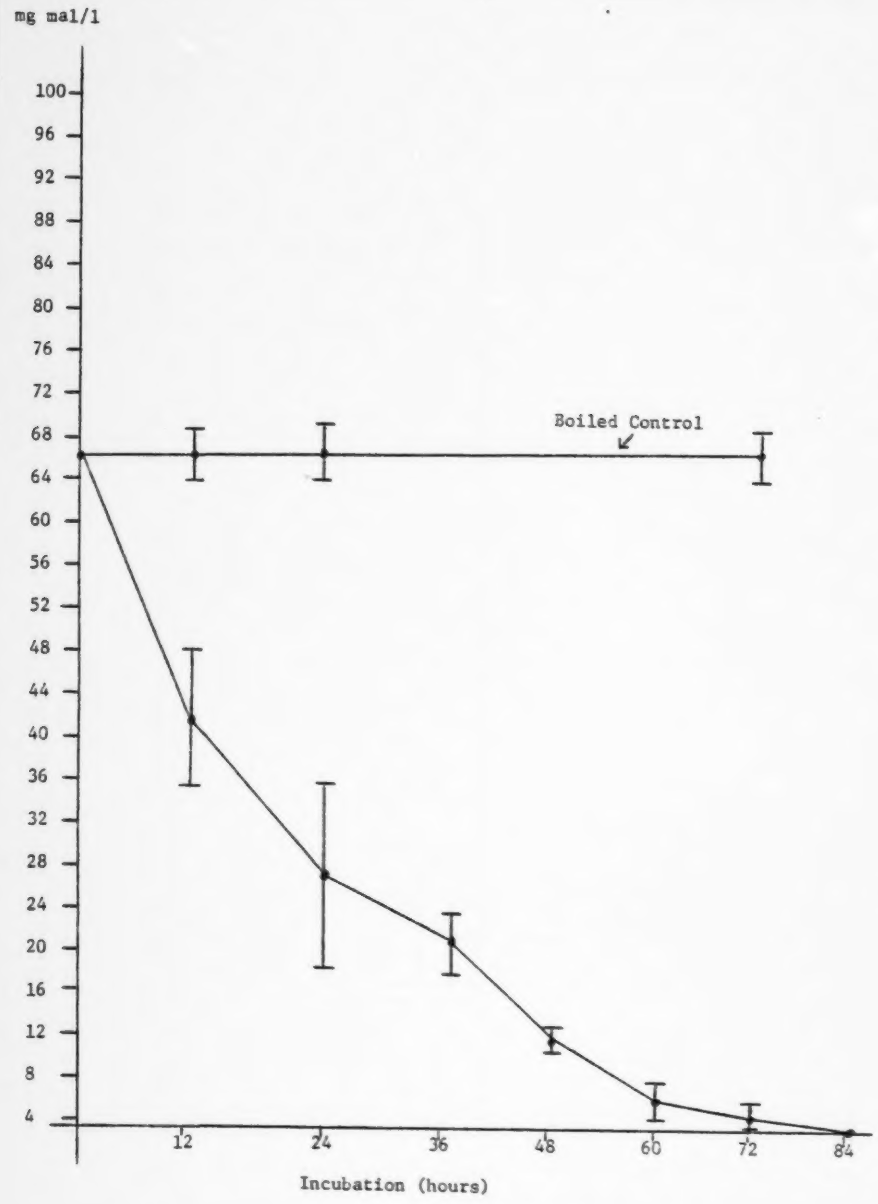

Figure 7. Malathion remaining vs. incubation time.

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(4-76)

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where

DO2 = dissolved oxygen concentration (g/m^3)
DOMIN = minimum effect under anaerobic conditions (unitless)
MKO2 = half-saturation constant for oxygen (g/m^3)

For aromatic compounds, no degradation of the aromatic ring occurs under anaerobic conditions. Side chains can, however, be degraded, e.g. the acetic acid moiety of 2,4-D; therefore, a minimum limit (DOMIN) is imposed on the reduction factor. Aerobic metabolism is practically independent of oxygen tension above a critical value (about 0.01 atm for pure cultures) (Figure 8).

Because of the environmental conditions and the array of metabolic types in a natural assemblage, the rate of non-aromatic degradation is probably independent of oxygen, with anaerobic utilization of TOM occurring when oxygen becomes limiting for aerobic metabolism. Therefore, DOMIN = 1.

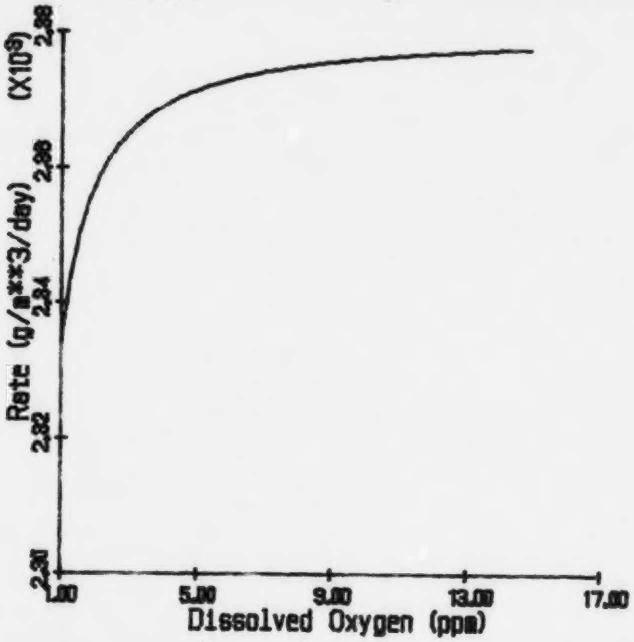

Figure 8. Effect of dissolved oxygen on microbial degradation of pentachlorophenol.

Most natural environments have pH values between 5 and 9 (Brock, 1970). Most bacteria grow best under neutral or slightly alkaline (pH 6.8-8) conditions, whereas most yeasts and fungi prefer slightly acidic environs (pH 5-6). Under otherwise optimal conditions, the pH response curve of a natural assemblage (of environmental pH 5-9) exposed to an instantaneous pH

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(4-76)

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shift can be represented by:

$$PHCOR = \begin{cases} KPH*e^{(pH-PHMIN)} & \text{if } pH \leq PHMIN \\ KPH*e^{(PHMAX-pH)} & \text{if } pH \geq PHMAX \\ 1 & \text{otherwise} \end{cases} \qquad \text{(Eq. 19c)}$$

where

KPH = adaptive constant for pH (unitless)
pH = pH
PHMIN = critically low pH
PHMAX = critically high pH

This can be parameterized to yield a broad peak reflecting the composite effect of many different organisms with differing pH optima within the 5-9 range (Figure 9).

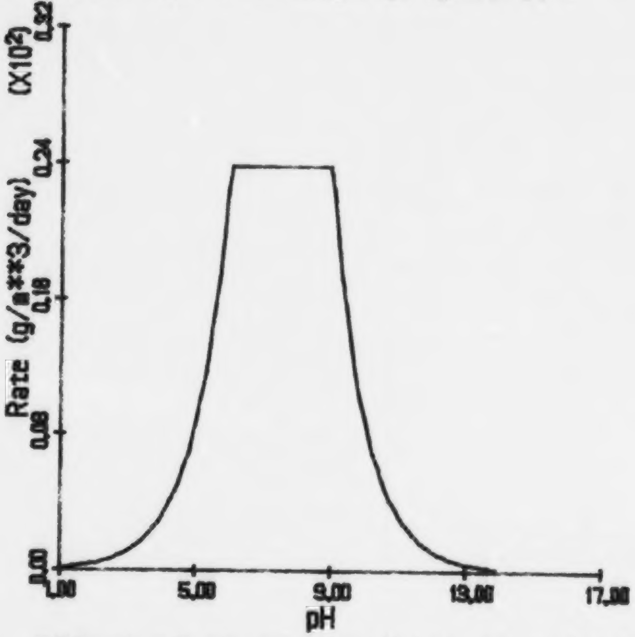

Figure 9. Effect of pH on microbial degradation of pentachlorophenol.

Given sustained conditions of pH values outside of the 5-9 range, restricted populations will develop that are tolerant of those conditions. Acidified lakes (pH 3.5) and mine drainage (pH 4.2), and alkaline lakes (pH 9.5) develop specialized microflora. Some of these organisms exhibit pH optima close to the pH of the environs and others are simply tolerant of those conditions. The population composition will be a reflection of the competition between the acidophilic or alkalophilic

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EPA-287 (Cin.)
(4-76)

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organisms and the tolerant organisms. The population density and growth rate however will not be as high as it would be if that same system were neutralized (e.g., dystrophic lake) since it is believed that microorganisms must expend energy in order to maintain their internal neutral conditions in an acid or basic environment. The overall effect is a broadening of the curve, but a lowering of the activity and density of the population. The KPH, PHMIN, and PHMAX parameters can be adjusted for these unusual conditions.

The temperature reduction factor is formulated similarly to that for pH to provide a plateau of adaptation (Figure 10):

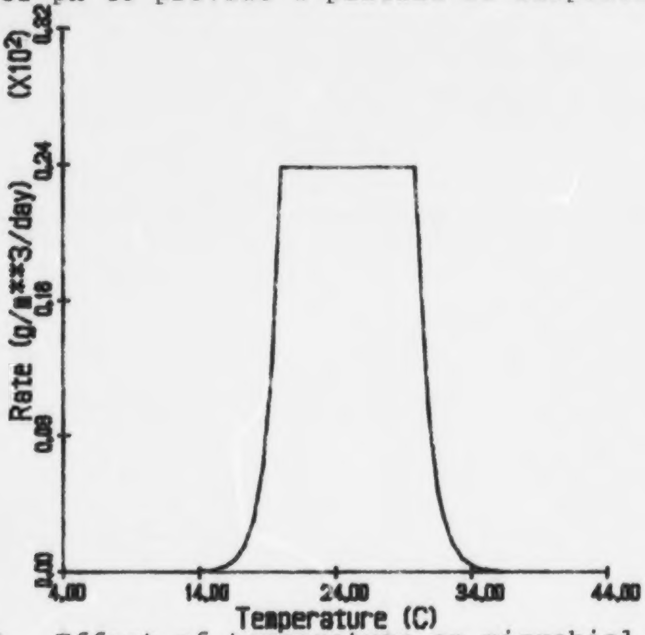

Figure 10. Effect of temperature on microbial degradation of pentachlorophenol.

$$\mathrm{TPCOR} = \begin{cases} \mathrm{KTP}*e^{(\mathrm{TEMP}-\mathrm{TPMIN})} & \text{if TEMP} \le \text{TPMIN} \\ \mathrm{KTP}*e^{(\mathrm{TPMAX}-\mathrm{TEMP})} & \text{if TEMP} \ge \text{TPMAX} \\ 1 & \text{otherwise} \end{cases} \qquad \text{(Eq. 19d)}$$

where

KTP = adaptive constant for temperature (unitless)
TEMP = ambient temperature (°C)
TPMIN = critically low temperature (°C)
TPMAX = critically high temperature (°C)

The usual range of temperature required for growth of a

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

given organism is 30-40 degrees. It is very rare that temperatures in nature exceed 50°C, especially in water (with the exception of hot springs). During seasonal variations in temperature, microbial populations in lake sediments maintain a temperature optimum corresponding to the maximum temperature attained by the lake or higher (Boylen and Brock, 1973). This may result in reduced decomposition activity during the periods when temperature is less than 25°C. The actual effect, however, will depend upon the controlling limiting variable for growth, i.e. growth may be greater at 10°C than 15°C if there is limiting energy subtrate at 15°C. Psychrophilic organisms that may develop are not abundant enough to affect the overall rate. In contrast, systems that are permanently cold or hot develop predominantely psychrophilic or thermophilic populations and TPMIN and TPMAX can be changed to reflect these unusual conditions.

Evidence from studies at Lake George, New York (Clesceri, Boylen and Park, 1977) has shown the direct effect of mixing on cellulose degradation. These studies were done in filled, closed flasks to separate the effect of aeration from agitation.

At the present time mixing is represented simplistically as a function of wind speed in PEST:

$$\mathrm{TMIX} = \begin{cases} \dfrac{\mathrm{WINDV}}{\mathrm{WMIX+WINDV}} & \text{if DPHLIM} < \text{DEPTH} \\ 0 & \text{if DPHLIM} \leq \text{DEPTH} \end{cases} \qquad \text{(Eq. 19e)}$$

$$\mathrm{DPHLIM = KDEPTH*WINDV} \qquad \text{(Eq. 19f)}$$

where

WMIX = windspeed at 1/2 maximum stirring effect (m/sec)
WINDV = windspeed (m/sec)
KDEPTH = constant relating wind energy to depth
DPHLIM = depth at which wind energy is unimportant (m)
DEPTH = depth of water (m)

The presence of other compounds has been shown to facilitate the metabolism of recalcitrant molecules (Horvath, 1972; Merkel and Perry, 1977). If natural inocula and associated substrates are used in the METMAX determination, it is likely that such cosubstrates will be present.

It is unlikely that an aquatic sediment will be deficient in mineral nutrient (eg. N,P) for the metabolism of the available energy substrates. Minerals are recycled within the sediment system which becomes enriched in these nutrients (Clesceri, Boylen, and Park, 1977). Our studies for the determination of METMAX for 2,4-D, atrazine and malathion with lake sediments have revealed no increase by the addition of inorganic nitrogen (as NO_3^- and NH_4^+ or inorganic phosphorus (as $H_2PO_4^-$).

The TADPT factor allows for the development of microbial biomass capable of TOM biodegradation. Adaptation may be genetic and occur through mutation or it may be the acquisition of new genetic elements (transmissible plasmids, Meynell, 1972). It may also be simply the time required for induction of suitable enzymes within the existing population. The factor is derived through the use of an adaptation potential which expresses whether or not the adaptation will occur during the time of exposure to TOM. If the adaptation time exceeds the exposure time, the adaptation potential has a fractional value, representing the fraction of potential TOM degraders present at that time. If the adaptation time is less than the exposure time the adaptation potential is 1. Thus the TADPT is determined by the microbial biomass in the system and the adaptive capability of the organisms:

$$\text{TADPT} = \text{BACB}*\begin{cases} 0 & \text{if } [\text{EXPT}/(\text{MMGT}*\text{STRU}*\text{A}] < 0 \\ 1 & \text{if } [\text{EXPT}/(\text{MMGT}*\text{STRU}*\text{A}] > 1 \\ \text{EXPT}/(\text{MMGT}*\text{STRU}*\text{A} & \text{otherwise} \end{cases} \qquad \text{(Eq. 19g)}$$

where

BACB = microbial biomass (g organism/m^3)
MMGT = generation time under METMAX conditions (day)
STRU = structural activity factor (unitless)
EXPT = time of exposure to TOM (days)

$$\text{EXPT} = \text{TIME-STTOM+1} \qquad \text{(Eq. 19h)}$$

where

TIME = Julian date in simulation
STTOM = Julian date of introduction of TOM

TADPT can be determined for a specific TOM along with the METMAX measurement. It can also be calculated for related compounds using the A term, the generation time of the assemblage under METMAX conditions (MMGT) and the structural factor (STRU).

Mutation rate is dependent on generation rate under most conditions, but observed to be independent of generation rate under amino acid- or nitrogen-limited conditions in continuous culture (Kubitschek and Bendigketi, 1961). In addition to the mutation rate, the ability to develop a biodegradation capability for a certain TOM depends on the structural factor (STRU) which may be estimated by means of structural activity

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EPA-287 (Cin.)
(4-76)

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relationships (Jaffe, 1953; Kapoor et al., 1973). Structure-activity studies developed for mammalian systems have a great deal of applicability to microbiological transformations. The concept that biological activity can be predicted from chemical structure is very old (Crum-Brown and Fraser, 1869). Expanding the distribution prediction based on partition coefficients (Leo, Hansch and Elkins, 1971) to include transformation prediction based upon substructural fragments seems feasible for ecosystems as well as animal systems.

SORPTION

SORP

The adsorption of TOM to the surfaces of the organic and inorganic components is treated with a relatively simple algorithm. However the approach is well grounded in physical chemistry. The initial calculation determines the amount of TOM both dissolved in the water and on the surfaces of the various components of the system:

$$\mathrm{TOTPST} = \sum_{I} \mathrm{CONCEN(I)*SAREA(I)} \qquad \text{(Eq. 20)}$$

where

TOTPST = the total concentration of TOM in the environment (grams TOM/m^3)
CONCEN(I) = the concentration of TOM in the Ith compartment (grams TOM/m^3)
SAREA(I) = the percentage of TOM in the Ith carrier at the surface (unitless)

The parameter SAREA is used to indicate that of the total concentration of toxic material only a fraction is actually at the surface of the organism or particle and thus available for the physical process of adsorption. This allows the representation of rapid initial adsorption to the surface to be separated from the slower migration of the TOM into the carrier, as noted by Kenaga and Goring (1980).

The second part of the sorption routine uses the octanol-water partition coefficient to indicate the equilibrium concentration in each carrier, assuming no limitation on the quantity of TOM available. This function:

$$\mathrm{NEWAMT(I) = KPART(I)*CONCEN(13)*LOAD(I)*SAREA(I)*1E\text{-}6} \qquad \text{(Eq. 21)}$$

where

NEWAMT(I) = the equilibrium concentration for the Ith carrier (ppm)
KPART(I) = the octanol-water partition coefficient for the

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EPA-287 (Cin.)
(4-76)

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TOM being modeled and the Ith carrier
CONCEN(13) = the concentration of TOM in the water (g/m^3)
LOAD(I) = the mass concentration of the Ith carrier (g/m^3)

calculates the concentrations in units of parts per million and again utilizes the parameter SAREA to indicate only the surface of the carrier is involved in this process.

The final concentrations, after adsorption has occurred is calculated:

$$\text{CONCEN(I)} = \text{NEWAMT(I)}* \frac{\text{TOTPST}}{\sum_{I}\text{NEWAMT(I)}} + \text{OLDAMT(I)} \qquad \text{(Eq. 22)}$$

where

CONCEN(I) = the new concentration of TOM in each Ith carrier (g TOM/m^3)
OLDAMT(I) = the concentration of TOM within the carrier, not affected by adsorption (g/m^3)

The middle term in this function is used to normalize the amount of adsorption taking place so that mass balance is maintained.

This sorption algorithm differs from the others of the PEST model in that it returns a concentration rather than a rate. This is because the rate at which TOM adsorbs to a surface is at a time scale much shorter than that at which the model runs (Kenaga and Goring, 1980; Kenaga, 1975; Haque, 1974) and can therefore be represented as occurring instantaneously.

GILL SORPTION GILSRP

The major route of uptake of TOM by fish has been considered to be the result of active transport through the gills (Macek, et al., 1977). As the organism respires, water is passed over the outer surface of the gill and blood is moved through the inner surface. The exchange of TOM through the gill membrane is assumed to be facilitated by the same general mechanism as the uptake of oxygen and release of carbon dioxide, following the approaches of Fagerstrom and Åsell (1973, 1975) and Weininger (1978).

The formulation developed to calculate the uptake of TOM by the gills was designed to represent the actual pathways of accumulation. Assuming a lipophilic material (although that assumption is not necessary, non-lipophilic materials can be represented as well) we can conceptualize an organism as having three areas of import to this process: fat depots where the

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

material is stored, the gill membrane, and blood which provides the link between the two. The flow of TOM can then be thought of as first from the water through the gill membrane and into the blood and then from the blood into the fat where it accumulates.

To represent this process we must know the relative concentrations of toxic material in the water and in the blood and their variance from the equilibrium concentrations. The amount of TOM transferred would be a function of this partitioning and the partitioning between the blood and the fat. The rate at which the TOM is transferred would be a function of the efficiency with which the material could be passed through the gill to the blood and the rate of blood circulation to move the material to the fat. To calculate the gradient along which the TOM will move, the concentrations on each side of the gill membrane must be calculated. To find the concentration in the blood the respiration rate is calculated using a function developed for the MS.CLEANER ecosystem model (Park et al., 1980):

$$\begin{aligned} \mathrm{CRS(J)} = {} & \mathrm{EXP(KTEMP(J)*(TEMP-TOPT(J))*RMAX(J)} \\ & \mathrm{*BIO(J)+(KRESP(J)*(\Sigma CTWO(J)-\Sigma DTWO(J)))} \end{aligned} \qquad \text{(Eq. 23)}$$

where

CRS(J) = the rate of biomass loss due to respiration (g/m^3 day)
KTEMP(J) = a coefficient describing rate of increase of respiration with temperature (1/°C)
TEMP = the water temperature (°C)
TOPT(J) = the optimum temperature for respiration (°C)
RMAX(J) = the respiration rate at starvation (g/g/day)
BIO(J) = the biomass of the Jth organism (g/m^3)
KRESP(J) = a coefficient relating respiration to metabolism
ΣCTWO(J) = the total rate of consumption by the Jth organism (g/m^3 day)
ΣDTWO(J) = the total rate of defecation by the Jth organism (g/m^3 day)

The concentration that passes through the gills in the blood, BCIRC (in g TOM/m^3 day), is calculated by:

$$\mathrm{BCIRC(I)} = \frac{\mathrm{CRS(I)*O2RESP(I)*CONCEN(I)}}{\mathrm{BLDO2(I)*PCBLD(I)*PCFBL*BIO(J)*PCFAT(I)}} \qquad \text{(Eq. 24)}$$

where

O2RESP(I) = coefficient relating oxygen uptake to respiration (g O2/g biomass)

EPA-287 (Cin.)
(4-76)

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PCFBL = fat/blood partition coefficient (assumes the TOM is concentrated in the fat, i.e., lipophilic
CONCEN(I) = concentration of TOM in Ith organism (g TOM/m^3)
PCFAT(I) = percent fat in the Ith organism (g fat/g biomass)
BLDO2(I) = coefficient for oxygen capacity of blood (g O_2/g blood)
PCBLD(I) = percent blood (g blood/g biomass)

The volume of water processed is also calculated as a function of the respiration rate, CRS, and used to determine the amount of TOM in the water that passes through the gill. WCIRC (g TOM/m^3 water processed day) is calculated as:

$$\mathrm{WCIRC(I)} = \frac{\mathrm{CRS(I)*O2RESP(I)*CONCEN(13)}}{\mathrm{DO2}} \qquad \text{(Eq. 25)}$$

where

CONCEN(13) = concentration of TOM in the water (g TOM/m^3)
DO2 = concentration of dissolved oxygen in the water (g O_2/m^3)

The total "exposure" of the blood of the organism to the TOM must be checked to prevent the inclusion of more TOM than is present in the system. This check is necessitated because an organism may circulate its entire blood supply through its gills many times per day (Nicol, 1960) and because gill sorption is assumed to occur almost instantaneously.

To calculate the exchange of TOM the gradient between the concentrations in the blood and water must be established. Since the toxic material will tend to adsorb onto organic particles and this activity can be related to a partition coefficient (Kenaga, 1975; Chiou et al., 1977), the gradient along which the material will move can be calculated using this coefficient. The formulation is:

$$\mathrm{DIR(I) = WCIRC(I)*PCBLW-BCIRC(I)} \qquad \text{(Eq. 26)}$$

where

DIR(I) = the difference in concentrations (g TOM/m^3 day)
PCBLW = the partition coefficient for blood to water for the particular TOM

The blood-water partition coefficient, PCBLW, and the fat-blood partition coefficient, PCFBL, are used to represent the series of partitionings from the water to the lipid (Kapoor et al., 1973) as noted in the description of the conceptual basis of the function. If the particular TOM being modeled is not lipophilic the fat-blood partition coefficient is not necessary and may be set equal to one. The values for these

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(4-76)

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coefficients may be determined experimentally or may be calculated (Leung, 1978).

The total of the differences between equilibrium and present levels in each organism is summed and used to normalize the rate of gill sorption:

$$\mathrm{NORM} = \frac{\sum_{I} \mathrm{BCIRC(I)} + \sum_{I} \mathrm{WCIRC(I)}}{\sum_{I} \mathrm{DIR(J)}}$$

This normalization insures the maintenance of mass balance and is necessary due to the instantaneous nature of the actual process of sorption as opposed to the sequential calculations.

The actual rate of gill sorption, GILSRP (g TOM/m^3 day), is calculated by:

$$\mathrm{GILSRP(I) = EFFEN(I)*DIR(I)*NORM} \qquad \text{(Eq. 27)}$$

where

EFFEN(I) = a coefficient describing the efficiency of the gill membrane in the transport of the TOM through it (unitless)

The efficiency coefficient, EFFEN, is used to modify the rate to comply with the assumption basic to the formulation: the transport of TOM is facilitated by the same general mechanism as oxygen. This coefficient is similar to that of Weininger (1978) in that it compares the diffusivity of the toxic material being modeled with that of oxygen and modifies the predicted rate of gill sorption to account for this difference.

The final calculation of this function is the subtraction of each individual rate from the concentration in the water to maintain mass balance. To illustrate the response of this process with time of exposure, gill sorption was calculated assuming a constant 3.0 ppm in the water, a basal respiration rate, and constant biodegradation. The response is illustrated in Figure 11 and is compared with the data of Lockhart et al., (1977).

CONSUMPTION

CONS

This routine calculates the rate of change in the TOM concentration of an organism as the result of ingestion, defecation, and excretion. The effects of these individual processes are added to obtain a single rate, CONS, in units of g TOM/m^3 day.

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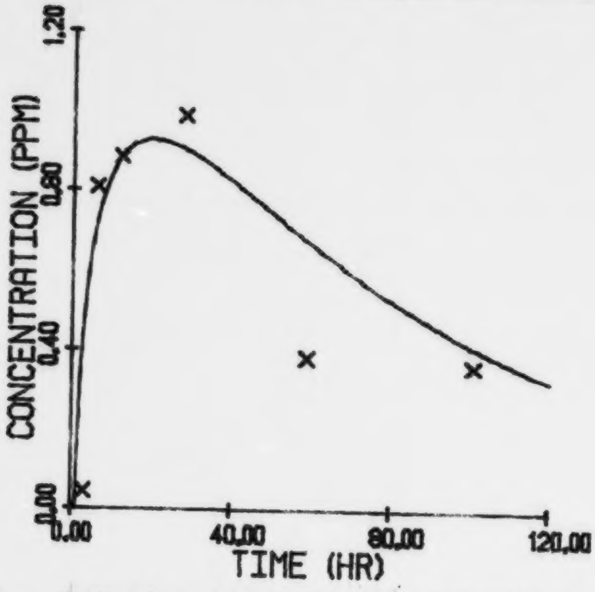

Figure 11. Relation between the concentration of methoxychlor in a fish and time. Data points are averages from measurements of Lockhart et al., 1977.

9-1/8"

Ingestion

The rate of ingestion is calculated primarily as a function of the biomass concentrations of prey I and predator J, which are supplied to the model as driving variables. The predators may follow one of three general strategies for ingestion as indicated by the parameter FEDSWT: FEDSWT=0 indicates carnivores; FEDSWT=1 indicates filter-feeders; and FEDSWT=2 indicates filter-feeding, benthic organisms that produce pseudofeces. Carnivores and non-depositing filter-feeders both utilize a saturation-kinetic equation, modified from CLEANER (Scavia and Park, 1976).

For carnivores ingestion of biomass is calculated as:

$$\mathrm{CTWO} = \frac{\mathrm{CMAX(J)*W(I,J)*BIO(I)*BIO(J)*LIM*TRED*O2COR}}{\mathrm{Q(J)}+\sum_{\mathrm{I}}\mathrm{(W(I,J)*BIO(I))*LIM}} \qquad \text{(Eq. 28)}$$

where

CTWO = the ingestion of prey I by predator J (g/m^3 day)
CMAX = the maximum rate of ingestion (g/g day)
W(I,J) = the preference for prey I by predator J (unitless)
BIO(I) = the biomass concentration of the Ith prey (g/m^3)

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3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

BIO(J) = the biomass concentration of the Jth predator (g/m^3)
Q(J) = the half-saturation constant for feeding (g/m^3)

The three terms LIM, O2COR, and TRED are correction functions. LIM (Leung et al., 1978) is used to indicate reduction in ingestion rate due to low prey concentrations:

$$\mathrm{LIM} = 1.0-(\mathrm{BMIN(J)}/\sum_{\mathrm{I}}\mathrm{BIO(I)}) \qquad \text{(Eq. 29)}$$

where

BMIN(J) = the prey concentration at which the predator begins feeding (g/m^3)

The reduction of ingestion rate that results from low dissolved oxygen concentrations is calculated by the function O2COR (Park et al., in prep.):

$$\mathrm{O2COR} = \mathrm{DO2}/(\mathrm{KO2(J)}+\mathrm{DO2}) \qquad \text{(Eq. 30)}$$

where

DO2 = the dissolved oxygen concentration (g/m^3)
KO2(J) = the saturation coefficient for oxygen limitation (g/m^3)

TRED is the reduction factor for non-optimal temperature, originally developed by O'Neill et al. (1972) and modified by Scavia and Park (1976) for application to aquatic ecosystems. It is formulated to reflect the response of organisms to variations in temperature as:

$$\mathrm{TRED} = \mathrm{V}^{\mathrm{X}} * e^{(\mathrm{X}*(1-\mathrm{V}))} \qquad \text{(Eq. 31a)}$$

$$\mathrm{V} = \frac{\mathrm{TMAX-T}}{\mathrm{TMAX-TOPT}} \qquad \text{(Eq. 31b)}$$

$$\mathrm{X} = \frac{w*[1+(1+\frac{40}{w})^{.5}]^{2}}{400} \qquad \text{(Eq. 31c)}$$

$$w = \ln(\mathrm{Q10})*(\mathrm{TMAX-TOPT}) \qquad \text{(Eq. 31d)}$$

where

TMAX = the maximum temperature at which process will occur (°C)
TOPT = the optimum temperature (°C)
Q10 = the rate of change per 10°C temperature rise (unitless)
T = the water temperature (°C)

The calculation of ingestion by saturation-type filter-feeders is accomplished by replacing the maximum consumption rate parameter, CMAX, with a maximum filtering rate, FMAX (g filtered/g day).

The production of pseudofeces by filtering organisms is calculated in three steps (Albanese, 1979). First the water processing rate:

$$FIL = FMAX(J)*TRBRED*(\sum_{I} BIO(I)-BMIN(J))/(Q(J)+\sum_{I} BIO(I)-BMIN(J)) \qquad \text{(Eq. 32)}$$

where

FIL = the rate of filtering (g/g day)
TRBRED = a reduction factor for filtering rate due to high concentration of inorganic particles

and the other parameters as previously defined are calculated. The second process, that of biodeposition, is calculated as:

$$BIODEP = EXP(BDSLP(J)*BIO(I)-BDINT(J)) \qquad \text{(Eq. 33)}$$

where

BIODEP = the rate of production of pseudofeces (g/g day)
BDSLP(J) and BDINT(J) = regression coefficients relating biodeposition to food concentration

The rate of ingestion is then the difference between the filtering rate and the biodeposition rate.

The ingestion of TOM is calculated using the rate of ingestion of biomass and the concentration of TOM in each prey:

$$CPTWO = CTWO*CONCEN(I)/BIO(I) \qquad \text{(Eq. 34)}$$

where

CPTWO = the rate of ingestion of TOM by each predator (g TOM ingested/m^3 day)
CONCEN(I) = the concentration of TOM in prey I (g toxic/m^3)

The defecation of TOM is then calculated:

$$DEF1 = CPTWO*E(I,J) \qquad \text{(Eq. 35)}$$

where

DEF1 = the rate of defecation of TOM (g/m^3 day)

E(I,J) = the percentage of TOM in the Ith prey that is egested by the Jth predator

The TOM that is biodeposited by filter-feeders is added to that produced by defecation and both are transferred to the particulate state-variable compartment. The rate of ingestion of prey I by predator J, CTWO, is also used to calculate the rate of TOM lost by the prey as the result of grazing by summing CPTWO by I, assuming that the total consumption must equal the total grazing.

The loss of TOM through excretion is calculated as a function of the respiration rate:

$$EX(J) = CRS(J)*KEXCR(J) \qquad \text{(Eq. 36)}$$

where

EX(J) = the rate of excretion of TOM by the Jth organism (g/m^3/day)
CRS(J) = the respiration rate (see GILSRP)
KEXCR(J) = a coefficient relating excretion to respiration (unitless)

If the TOM being modeled is lipophilic, the rate of release by excretion must be corrected as the fat reserves, having the highest TOM concentrations, would be utilized first. The correction factor for this is based on the ratio of the predicted ingestion rate to the maximum ingestion rate, which is supplied as either CMAX for FMAX depending on the feeding strategy of organism. As this ratio increases the organism is assumed to increase its fat content from the basal level as given by PFTBOD at the rate, FATRAT. In this way the condition of the organism is accounted for in the calculation of TOM released.

The calculated rates of ingestion, defecation, and excretion are then combined and passed to obtain the value of CONS.

BIOTRANSFORMATION BTRANS

This routine predicts the rate of biotransformation of the TOM to its daughter products; for some compounds it is a significant process of degradation (Khan et al., 1972). The rate is a function of the length of exposure to the TOM, the ambient temperature, and the concentration of the TOM in the organism.

$$BTRANS = \frac{MAX*CONCEN(I)}{KBTRAN(I)+CONCEN(I)} \qquad \text{(Eq. 37)}$$

EPA-287 (Cin.)
(4-76)

where

MAX = the maximum rate of biotransformation under the present environmental conditions (g transformed/g biomass day)
CONCEN(I) = the concentration of TOM in the Ith organism (g TOM/m^3)
KBTRAN(I) = the half-saturation coefficient for biotransformation (g TOM/m^3)

The rate of biotransformation is reduced for low metabolic capacity and for suboptimal temperature:

$$MAX = BTMAX*METCAP(I)*TRED \qquad \text{(Eq. 38)}$$

where

BTMAX = maximum rate of biotransformation (g transformed/g biomass day)
TRED = reduction factor for temperature (see Eq. 31a) (unitless)
METCAP(I) = the percent metabolic capacity for degradation of the TOM (unitless)

$$METCAP(I) = (TIME-STTOM+1)/BTTIM(I) \qquad \text{(Eq. 39)}$$

where

TIME = the day of the year (Julian date)
STTOM = the Julian date of introduction of the TOM to the environment
BTTIM(I) = the number of days required to reach full metabolic capacity

The relationship of this function to concentration is illustrated in Figure 12.

EPA-287 (Cin.)
(4-76)

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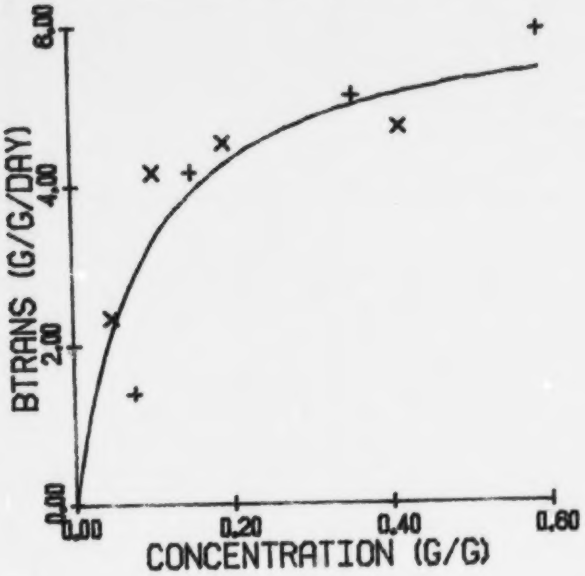

Figure 12. Relationship between BTRANS (g transformed/g organism/day) and TOM concentration (g TOM/g). Data are for aldrin epoxidation in bluegill fry (+) and in adult bluegills (X) (Stanton and Kahn, 1973).

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3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

SECTION 3

DATA REQUIREMENTS

Data requirements depend on the intended use of the model. If PEST is to be used as an evaluative model, as originally intended, then default data on prototype sites (such as the verification sites) may be sufficient to characterize the behavior and fate of a toxic organic material; therefore, site data would be unnecessary. If the model is to be applied as a diagnostic tool in order to better understand the fate of a compound at a particular site, then an accurate characterization of the site is required. If the problem involves bioconcentration in a particular group of organisms, then it will be necessary to accurately characterize the metabolic requirements and feeding preference of the organism.

COMPOUND-SPECIFIC PARAMETERS

To characterize all types of compounds for simulation by PEST, the following parameters are of interest. However, for a given compound some parameters, such as quantum yield for sensitized photolysis, may not be applicable or may be unavailable. The user of the model should exercise discretion in determining what parameters are necessary for a particular compound. Some parameters, such as the Henry's Law constant, can be derived from first-principle relationships and are calculated in PEST. For many parameters, use of a zero value will have the effect of cancelling a term in a process equation. The parameters for characterization of a compound include:

1. Hydrolysis

EN	activation energy for effect of temperature (cal/mole) p. 7
KA	rate constant for Bronsted acid catalysis (1/days) pp. 7, 11
KB	rate constant for Bronsted base catalysis (1/days) pp. 7, 11
KCAL	rate constant to account for colloidal, metal-ion, and phase-transfer catalysis (1/days) pp. 7, 12

KH	acid-catalyzed rate constant (l/M days) pp. 7, 9
KO	uncatalyzed rate constant (l/days) pp. 7, 9, 11
KOH	base-catalyzed rate constant (l/M days) pp. 7, 9, 11
TCOPT	temperature at which rate constant was obtained (°K) p. 7

2. Oxidation

KEFF	rate of radical initiation reaction, p. 15
KP	rate of reaction between TOM and alkoxy and peroxy radicals (l/day) p. 15
KT	rate of competing reaction between two radicals resulting in non-radical products (l/day) p. 15

3. Photolysis

ELAM	molar extinction coefficient for TOM at each wavelength (l/mole cm) p. 17
FRACD	fraction of irradiance that is direct at each wavelength (unitless) p. 17
FRACS	fraction of irradiance that is indirect at each wavelength (unitless) p. 17
KMEAS	rate constant for sensitized photolysis (l/day) pp. 20, 21
KSEN	empirical rate constant for sensitized photolysis (l/day) pp. 16, 20
PSIA	direct photolysis quantum yield for the TOM (unitless) pp. 16, 17
PSIB	sensitized photolysis quantum yield for the TOM (unitless) p. 16

4. Volatilization

HENRY	Henry's Law constant (atm.cm^3/mol) pp. 26, 27
KLEXPT	correction factor for volatilization (unitless) p. 24 (an empiricism to provide greater precision where necessary)
VPRESS	vapor pressure (atm) p. 26
VTOM	molal volume of TOM (cm^3/mol) pp. 26-28

5. Solution

SOLUB	solubility (mol/cm^3) pp. 26, 31

6. Microbial Degradation

KS	half-saturation constant for microbial metabolism (g/m^3) p. 32
METMAX	maximum rate of microbial metabolism (1/day) pp. 32, 33
STRU	structural activity factor for microbial degradation (unitless) pp. 39, 40

7. Sorption

KPART	octanol-water partition coefficient (unitless) p. 40

8. Bioaccumulation

BTMAX	maximum rate of biotransformation (g/g biomass day) p. 49
BTTIM	number of days required to reach full metabolic capacity (day) p. 49
E	percentage of TOM in prey that is egested (unitless) pp. 47, 48
EFFEN	coefficient for diffusivity of TOM through gill membrane (unitless) p. 44
EX	rate of excretion of TOM by each organism (g/m^3 day) p. 48
KBTRAN	half-saturation coefficient for biotransformation (g TOM/m^3) p. 49
PCBLW	blood:water partition coefficient, p. 43
PCFBL	fat:blood partition coefficient, p. 43

SITE-SPECIFIC CONSTANTS AND DRIVING VARIABLES

In order to run the model for a particular site, other than the representative prototype sites, it is necessary to have values for the following site characteristics:

ALPHA	extinction coefficient for site water at each wavelength (1/cm) pp. 17-20
CONCEN	initial concentration of toxic organic material (g/m^3) p. 7
D	median depth of water (cm) pp. 17, 18
DEPTH	depth of water (m) p. 38
HA	concentration of Bronsted acid (g/m^3) p. 7
HB	concentration of Bronsted base (g/m^3) p. 7
RAD	concentration of radical initiator present, p. 15

STTOM	Julian date of introduction of TOM, pp. 39, 49

Because PEST is a dynamic, time-varying model, it is also necessary to have time series of data for driving variables for the time period being simulated. The driving variables are:

BACB	microbial biomass (g/m^3) p. 39
BIO	biomass of each organism (g/m^3) pp. 42, 45
DO2	dissolved oxygen concentration (g/m^3) pp. 35, 43, 46
IIMEAS	observed light intensity (photons/cm) pp. 20, 21
LOAD	concentration of each carrier (g/m^3) pp. 40, 41 (= BIO)
pH	ambient pH, pp. 7, 13, 36
T	water temperature (°C) (= TEMP) p. 46
TEMP	ambient temperature (°C) pp. 7, 26, 37, 42
WINDV	wind velocity (m/sec) pp. 26, 38

ORGANISM-SPECIFIC PARAMETERS

The following information is desirable for adaptation of the bioaccumulation submodel for particular species:

BDINT	coefficient for biodeposition (unitless) p. 47
BDSLP	coefficient for biodeposition (unitless) p. 47
BIODEP	rate of production of pseudofeces (g/g day) p. 47
BLDO2	coefficient for oxygen capacity of blood (g O2/g blood) p. 43
BMIN	the prey concentration at which predator begins feeding (g/m^3) pp. 46, 47
CMAX	maximum rate of ingestion (g/g day) p. 45
FIL	rate of filtering (g/g day) p. 47
KEXCR	proportionality coefficient for excretion as a function of respiration (unitless) p. 48
KO2	saturation coefficient for oxygen limitation of ingestion (g/m^3) p. 46
KRESP	proportionality constant for respiration as a function of metabolism (unitless) p. 42
KTEMP	coefficient relating respiration rate to temperature (1/°C) p. 42
LIM	reduction in ingestion rate due to low prey concen-

	tration (unitless) pp. 45, 46
MAX	maximum rate of biotransformation under ambient environmental conditions (g/g biomass day) p. 49
O2RESP	coefficient relating oxygen uptake to respiration (g O2/g biomass) pp. 42, 43
PCBLD	percent blood (g blood/g biomass) p. 43
Q	half-saturation constant for feeding (g/m^3) pp. 45-47
Q10	rate of change per 10°C temperature change (unitless) p. 46
RMAX	respiration rate at starvation (g/g day) p. 42
SAREA	percentage of TOM at surface of carrier (unitless) p. 40
TMAX	maximum temperature at which process will occur (°C) p. 46
TOPT	optimum temperature (°C) pp. 42, 46
TRBRED	reduction factor in filtering rate due to high turbidity (unitless) p. 47
TRED	reduction factor for non-optimal temperature (unitless) pp. 46, 49
W	preference of predator for prey (unitless) p. 45

The following is needed to adapt the submodel for particular microbial assemblages:

DOCOR	reduction of microbial degradation due to suboptimal oxygen levels (unitless) p. 33
DOMIN	minimum value of oxygen reduction under anaerobic conditions (unitless) pp. 33, 35
KPH	adaptive constant for pH effect on microbial degradation (unitless) pp. 36, 37
KTP	adaptive constant for effect of temperature on microbial degradation (unitless) pp. 37, 38
MKO2	half-saturation constant for effect of oxygen on microbial degradation (g/m^3) pp. 33, 35
MMGT	microbial generation time under optimal conditions (days) p. 39
PHMAX	critically high pH for microbial degradation, pp. 36, 37
PHMIN	critically low pH for microbial degradation, pp. 36, 37
TMIX	reduction factor for effect of suboptimal mixing on microbial degradation (unitless) pp. 33, 38

TPCOR	reduction factor for effect of nonoptimal temperature on microbial degradation (unitless) pp. 37, 38
TPMAX	critically high temperature for microbial degradation (°C) p. 37

SECTION 4

VERIFICATION

Our philosophy of verification has been to use available parameter values, confirm the validity of the process equations by inspecting the process-response curves (such as are presented in the previous section), and then apply the model to the particular site without calibration. If the fit to the observed data was not acceptable the formulations were reexamined and improved, but the parameter values were not changed. This approach was taken because it was felt that there would not be opportunity or rationale for "fine-tuning" the parameter values in PEST using observed data when it was used as an evaluative model for new compounds.

However, in developing the model, this constraint proved to be frustrating. Correction of obvious deficiencies in the formulations sometimes led to worse fits to observed data. In fact, the simulations presented here represent just such a case; we discovered during the final stages of documentation that mass balance was not being maintained and that the TOM was being "lost" due to a programming error; we corrected the error and now the TOM does not disappear fast enough! This discrepancy in most of the simulations may indicate another problem in the formulations; or it may be a reflection of the uncertainty involved in the parameters for processes such as uptake by organisms, biotransformation, sensitized photolysis, and colloidal-catalyzed hydrolysis — these all tend to be conservative and lead to "worst case" simulations in the sense that the TOM is more persistent. There are also uncertainties involved in the driving-variable data and residue data for the sites. Therefore, the simulations can only be used to suggest that the model is behaving reasonably well. Unfortunately, the data are not sufficient for either validation or invalidation of PEST.

Based on our modeling experience, we recommend that future field verification studies include the following considerations:

- the mass (or biomass) of each carrier group,
- time series of TOM concentrations in the carriers,
- some idea of the bioenergetics of the biotic carriers

(such as consumption rates and prey preference), and

- enough information so that degradation pathways can be pinpointed (this could involve short-term use of radioactive-labelled material coupled with standard analytical determinations of TOM concentrations).

PARATHION IN ISRAELI FISHPONDS

As described by Perry and Gasith (1978), Parathion was introduced as a single 0.05 ppm application to each of two eutrophic fish ponds at Dor, Israel, on March 8, 1978; the experiment was concluded 67 days later. The ponds were 400 m^2 in area and averaged 1 m in depth. Data were given for concentrations in phytoplankton, zooplankton, waterbugs, benthic invertebrates (not modeled), carp, grass carp, silver carp, Tilapia, and water.

The driving variables and parameters used in the simulation are given in Appendix A. The principal source of uncertainty was in the diurnal variation of pH, which is very important in base-catalyzed hydrolysis of parathion (see Fig. 3a, p. 9). The simulation results are given in Figures 13a-e.

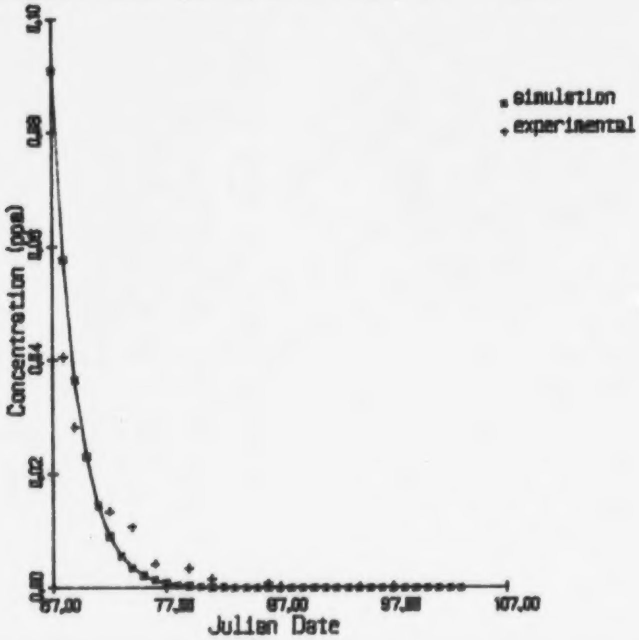

Figure 13a. Comparison of predicted and observed concentrations of Parathion in dissolved phase in Pond A-7, Dor, Israel. Data from Perry and Gasith, 1978.

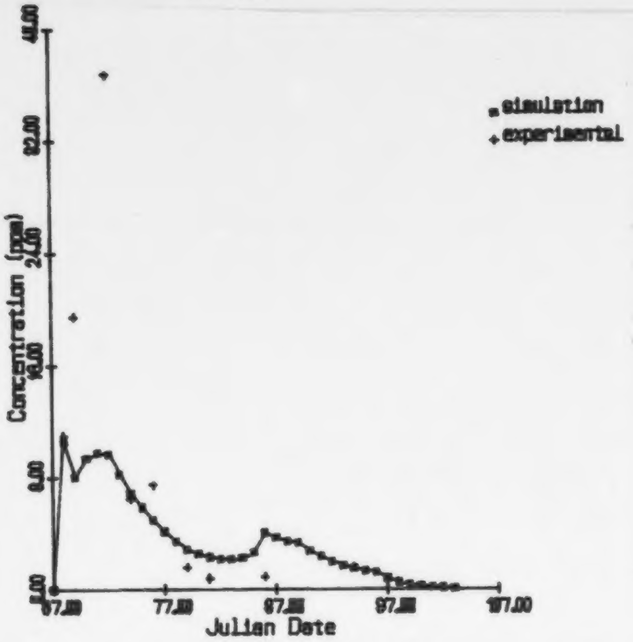

Figure 13b. Comparison of predicted and observed concentrations of Parathion in zooplankton in Pond A-7, Dor, Israel. Data from Perry and Gasith, 1978.

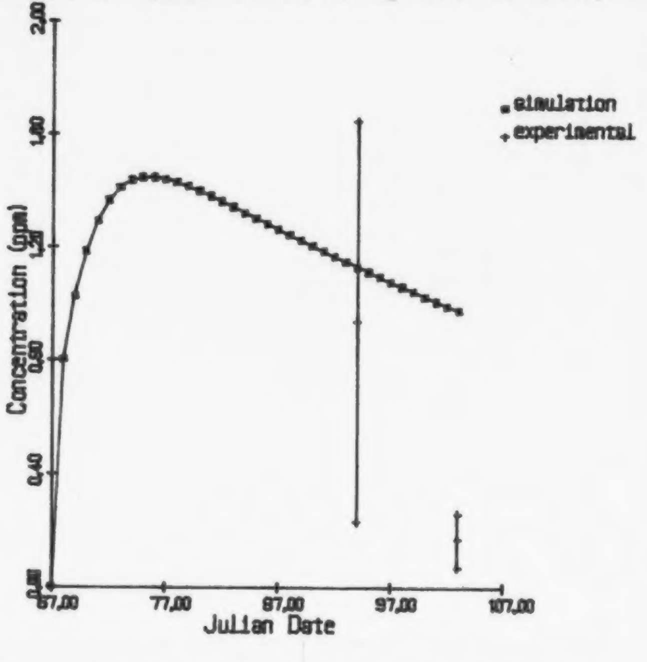

Figure 13c. Comparison of predicted and observed concentrations of Parathion in carp in Pond A-7, Dor, Israel. Data from Perry and Gasith, 1978.

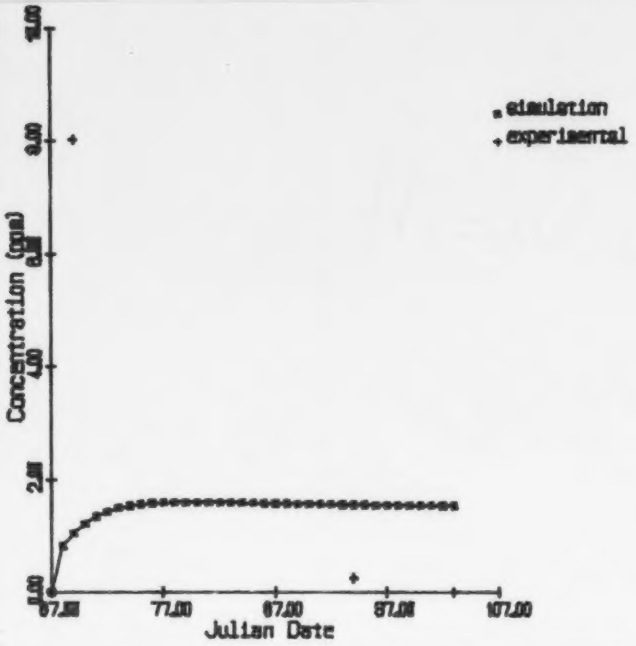

Figure 13d. Comparison of predicted and observed concentrations of Parathion in Tilapia in Pond A-7, Dor, Israel. Data from Perry and Gasith, 1978.

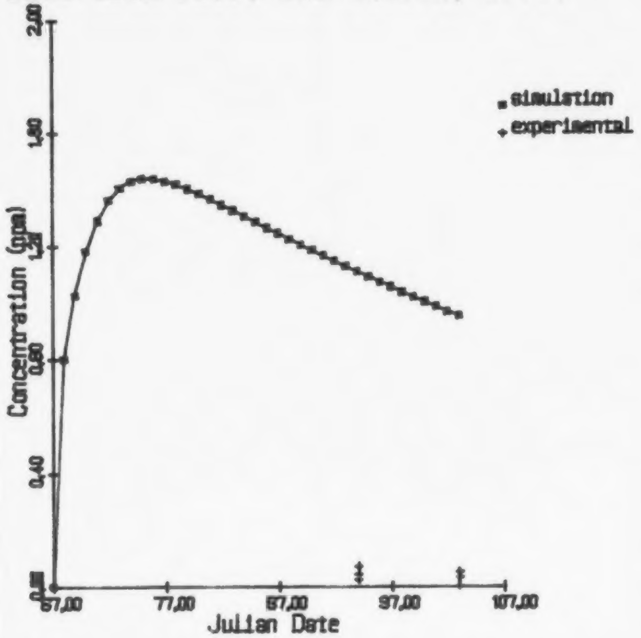

Figure 13e. Comparison of predicted and observed concentrations of Parathion in silver carp in Pond A-7, Dor, Israel. Data from Perry and Gasith, 1978.

PENTACHLOROPHENOL IN MISSOURI FISHPONDS

Pentachlorophenol was introduced as a single application of 1.0 ppm in each of 3 low-nutrient ponds without macrophytes at the Columbia, Missouri, National Fisheries Research Laboratory on May 22, 1978; the experiment was concluded 142 days later (T. P. Boyle and E. F. Robinson-Wilson, personal communication). The ponds were 297.28 m^2 in area and had an average depth of 1.20 m. Data were given for concentrations in large mouth bass and water.

The driving variables and parameters used in the simulation are given in Appendix B. The principal source of uncertainty was in the role of pH in the sediments as opposed to the water column; water-column values were used in the simulation, but the more acidic sediments may have been quite important due to the acid-catalyzed hydrolysis of Pentachlorophenol (see Fig. 3b, p. 10). Also, Pentachlorophenol degradation is sensitive to the effects of light attenuation on photolysis (see Table 6, p. 20). The simulation was further hampered by the availability of biomass data; the zooplankton values are only approximate conversions and the fish values were given only for the beginning and end of the experiment. The simulations are shown in Figures 14a-d.

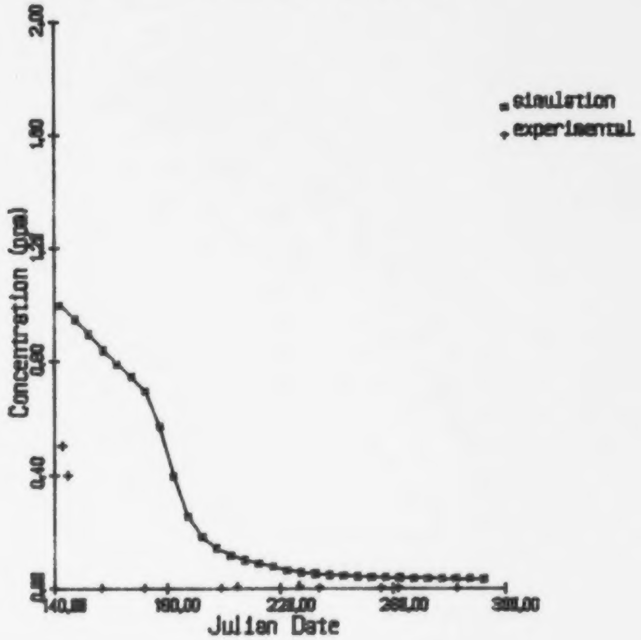

Figure 14a. Comparison of predicted and observed concentrations of Pentachlorophenol in dissolved phase in Treatment-3 ponds, Columbia, Missouri. Data from Boyle and Robinson-Wilson (unpub.).

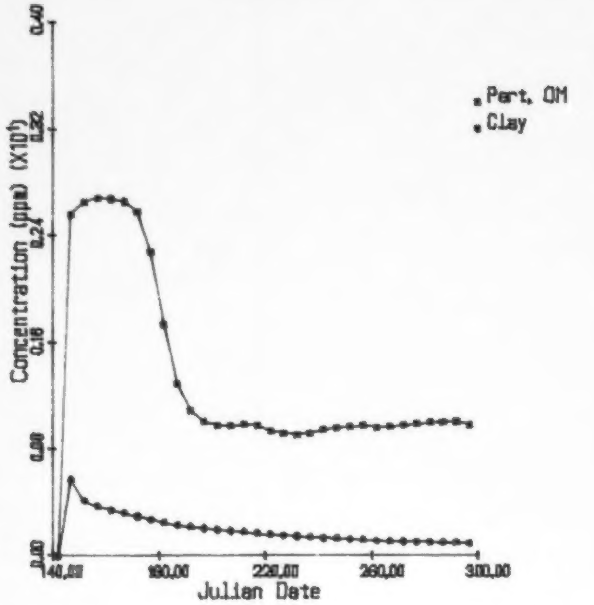

Figure 14b. Predicted concentrations of Pentachlorophenol in clay and particulate organic material in Treatment-3 ponds, Columbia, Missouri.

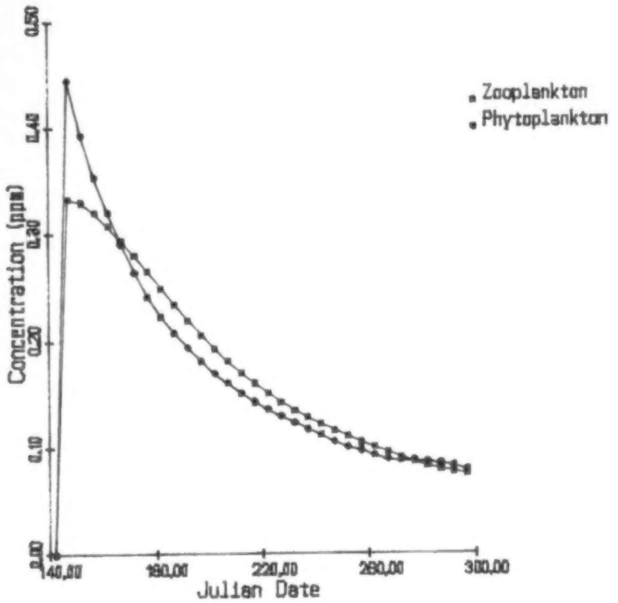

Figure 14c. Predicted concentrations of Pentachlorophenol in phytoplankton and zooplankton in Treatment-3 ponds, Columbia, Missouri.

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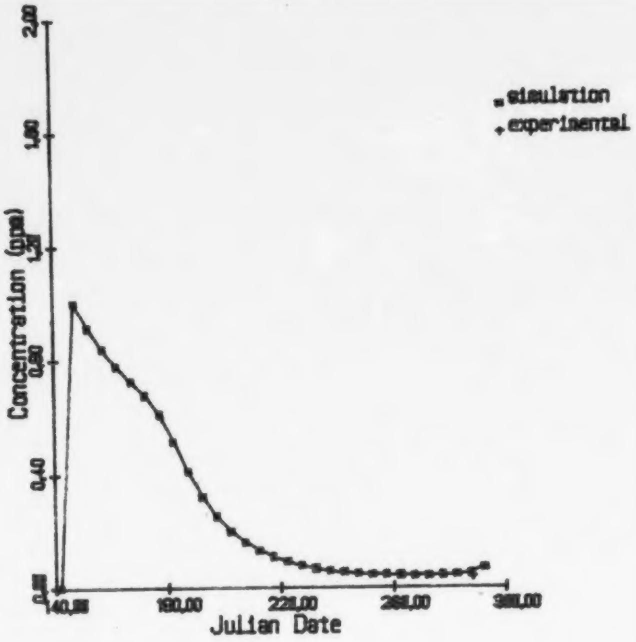

Figure 14d. Predicted and observed concentrations of Pentachlorophenol in large mouth bass in Treatment-3 ponds, Columbia, Missouri. Data from Boyle and Robinson-Wilson (unpub.).

In a concurrent treatment, Pentachlorophenol was introduced in 4 applications of 0.2, 0.2, 0.4 and 0.4 ppm in each of 3 low-nutrient ponds without macrophytes. The ponds were 297.28 m^2 in area and had an average depth of 1.48 m. Data were given for concentrations in bluegills, large mouth bass, channel catfish, and water.

The driving variables used in the simulation are given in Appendix C. The simulations are shown in Figures 15a-d.

DIELDRIN IN AN IOWA RESERVOIR

Dieldrin has been monitored in the Iowa River since 1968 and analyses for fish in Coralville Reservoir are available from 1970 to present; the compound has been quite persistent, although aldrin, its precursor, has been banned since 1975. Pesticide data summarized by Schnoor et al. (1979) and water quality data given by MacDonald (1079) were used in this study. The reservoir varies over 6 m in level; at conservation level the mean depth is 2.5 m. Maximum inflow in 1978 was 12,600 cfs; mean annual retention time is 14 days.

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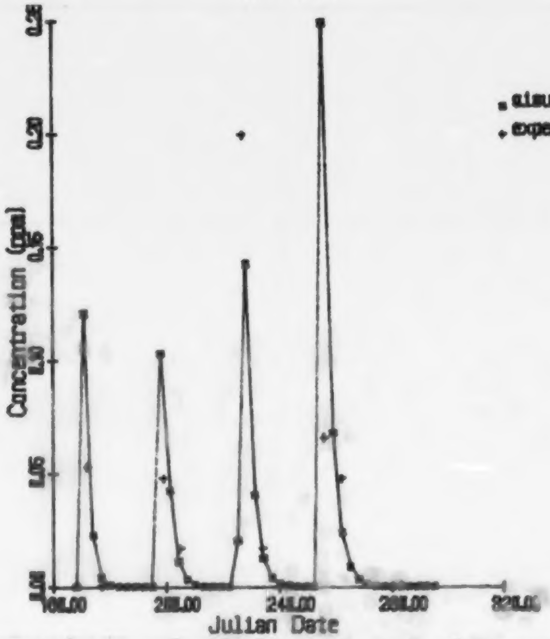

Figure 15a. Comparison of predicted and observed concentrations of Pentachlorophenol in dissolved phase in Treatment-2 ponds, Columbia, Missouri. Data from Boyle and Robinson-Wilson (unpub.).

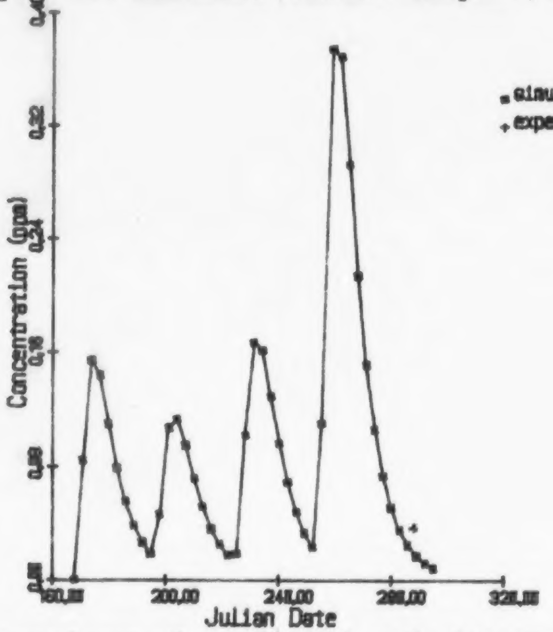

Figure 15b. Comparison of predicted and observed concentrations of Pentachlorophenol in bluegills in Treatment-2 ponds, Columbia, Missouri. Data from Boyle and Robinson-Wilson (unpub.).

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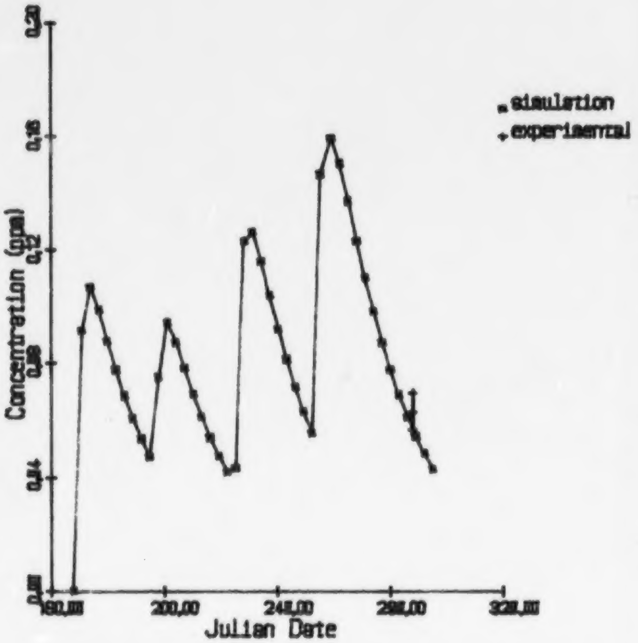

Figure 15c. Comparison of predicted and observed concentrations of Pentachlorophenol in large mouth bass in Treatment-2 ponds, Columbia, Missouri. Data from Boyle and Robinson-Wilson (unpub.).

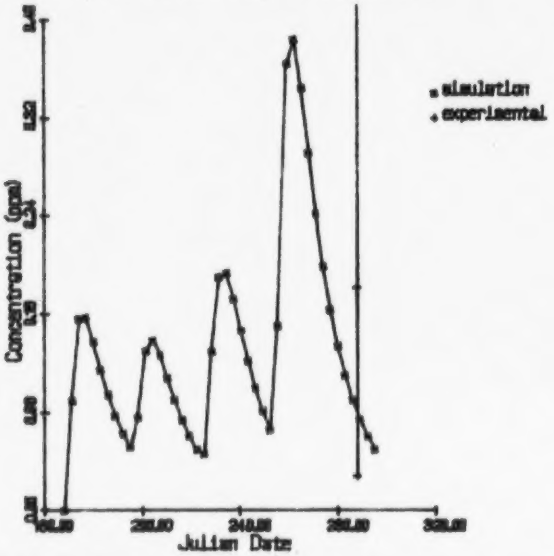

Figure 15d. Comparison of predicted and observed concentrations of Pentachlorophenol in channel catfish in Treatment-2 ponds, Columbia, Missouri. Data from Boyle and Robinson-Wilson (unpub.).

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The driving variables and parameters used in the simulation are given in Appendix D. Sources of uncertainty include the dieldrin loadings to Coralville Reservoir (downstream concentrations were used) and the biomass of organisms available to take up dieldrin. However, the simulations are clearly incorrect because outflow and sedimentation were not taken into consideration. We anticipate that later releases of the code will facilitate simulation of these important processes. The simulations are shown in Figures 16a and b.

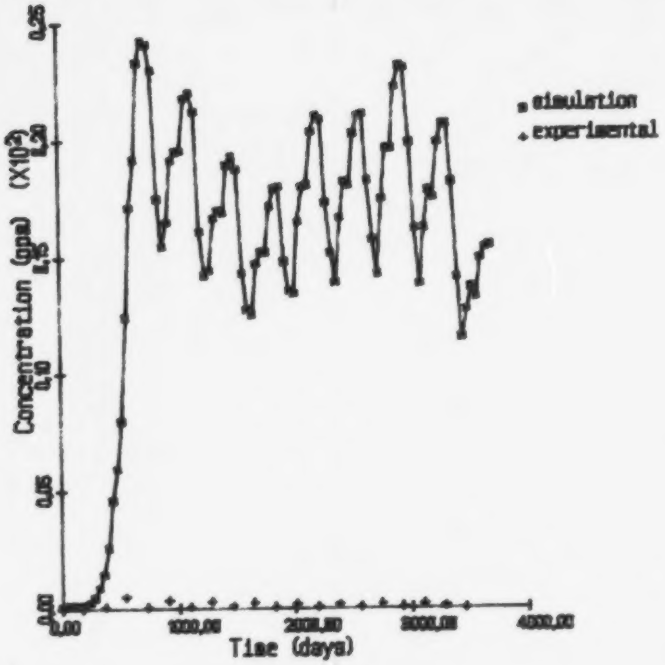


Figure 16a. Comparison of predicted and observed concentrations of Dieldrin in dissolved phase in Coralville Reservoir, Iowa from 1968 to 1977. Data from Schnoor et al. (1979).

However, when we used the sedimentation loss coefficient used by Schnoor (1979) the pattern of response was improved, but the results were still off by an order of magnitude (Figure 16c).

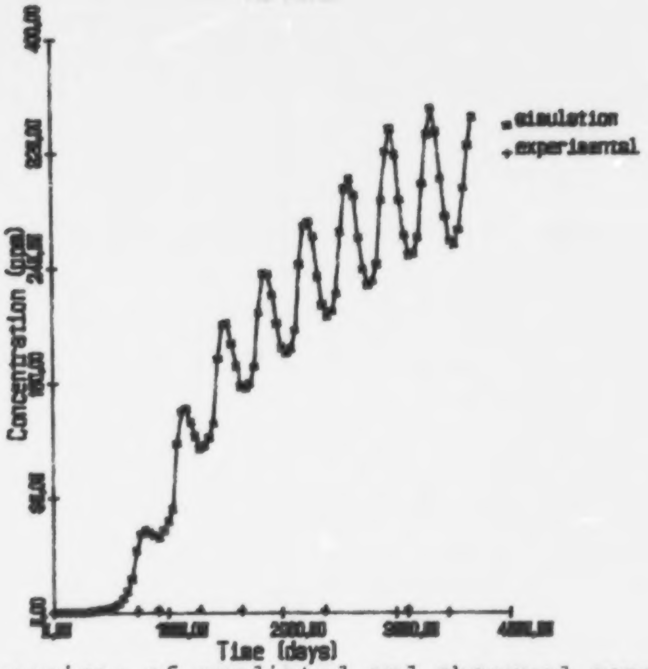


Figure 16b. Comparison of predicted and observed concentrations of Dieldrin in carp in Coralville Reservoir, Iowa.

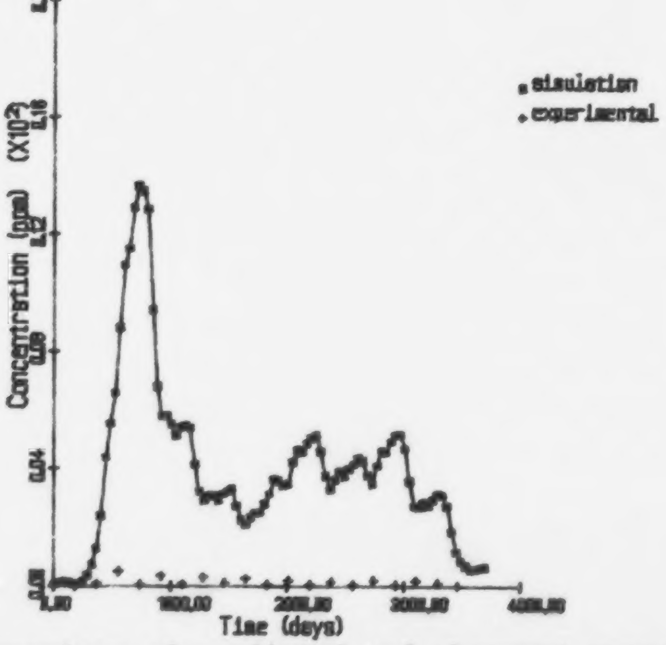


Figure 16c. Comparison of predicted and observed concentrations of Dieldrin in the dissolved phase in Coralville Reservoir, Iowa; sedimentation loss coefficient was used in the simulation.

SECTION 5

USER'S MANUAL

The PEST model is designed for interactive use, but can be used in a batch environment. There are ten commands in the model, including a HELP command that provides on-line assistance. "Yes?" is the prompt for a command.

LOGON

Having logged on to your system and begun execution of PEST, you will have to supply the name of the data file and indicate whether or not you are on a graphics device (DEC VT55 or similar).

Example

```
Are you on a graphics device? N
Name of parameter file:  PSPCP3.DAT
Yes?
```

EDIT

The EDIT command allows the user to edit any of the model's parameters, i.e., the data for the program. Because these data are in binary form, they cannot be altered using a conventional text editor, so this feature has been added to the model. The edit mode gives a "->" prompt to the user, after which an edit line may be entered. The EDIT mode is terminated by a ".".

Syntax

```
     EDIT
     <pname>=<value list> [,<pname>=<value list> ...]
  where
     <pname> is any variable listed in the parameter
     index file (I/O unit 10)

     <value list> is a list of one or more values to be
     assigned, or is an integer followed by an asterisk
     followed by a value to be assigned to the next n elements
```

of the parameter, or is an integer followed by an asterisk to display the next n values of the parameter

brackets indicate optional string of input

Examples

```
Yes?  EDIT
-> TLAST=*

TLAST=
   91
-> TFIRST=*

TFIRST=
   1
-> DO2=4*

DO2=
   11.50      10.40      3.900     3.000
-> DO2(2)=3*

DO2(2)=
   10.40      3.900     3.000

->DO2(3)=*, DO2(3)=4.00DO2(3)=*

DO2(3)=
    3.900

DO2(3)=
    4.00

->.
Yes?
```

START

The START command is the very heart of the model. This command causes a simulation to be performed. At the minimum, it will print a heading and a table of pesticide amounts according to day of simulation. Other information may be printed out depending on what previous commands the user may have entered (i.e., DEBUG and PRINT affect START's output). The heading contains the abbreviated state variable names (which may be altered by the EDIT command).

Syntax

START

Example

```
 Yes?  START
  Pesticide: DIELDRIN @CORALVILLE
--------------------------------------------------------------------
   TIME ZOOPL      WBUGS      CARP       PHYTO      WATER
--------------------------------------------------------------------
You did not start with equilibrium conditions.
 1:   1. 0.450     0.250       1.00      0.400      0.400E-05

 1:  31. 0.743     0.236       1.01      0.740      0.422E-05

 1:  64. 0.380     0.220      0.982      0.556      0.439E-05

 1:  94. 0.221     0.201      0.936      0.376      0.451E-05

Would you like a summary of the results ?  Y


 End of simulation.






     Summary of results:

                     Final amounts                         Half-life
Compartment       ppm             g/m**3         % Distrib.   (Days)
ZOOPL          .22092          .24688E-08      .23573E-01    16.000
WBUGS          .20128          .40255E-09      .38436E-02    16.000
CARP           .93617          .15827E-05      15.112        16.000
BUFALO         .92592          .20687E-05      19.752        16.000
CHCATF         .97330          .11165E-05      10.660        16.000
CRAPIE         .93695          .68054E-06      6.4978        16.000
WALEYE         .98941          .23922E-06      2.2841        16.000
<<8>>          .0              .0              .0            .0
<<9>>          .0              .0              .0            .0
<<0>>          .0              .0              .0            .0
PHYTO          .37638          .16149E-06      1.5419        16.000
MACRO          .30561          .43240E-07      .41286        16.000
WATER          .45103E-05      .45103E-05      43.064        .0
<FOM>          .0              .0              .0            .0
POM            .45944E-01      .45944E-07      .43867        16.000
CLAY           .43615E-01      .21807E-07      .20822        16.000
Initial amount of pesticide in ecosystem was .10393E-04 g/cubic meter.
Final   amount of pesticide in ecosystem  is .10473E-04 g/cubic meter.
```

PRINT

The user may wish to obtain output for state variables other than those included in the default table. PRINT will include or exclude a state variable from the output; the command acts as a toggle, reversing the print status of a state variable. Note that this does not exclude a state variable from the simulation! It is useful in limiting the output for small terminals. The command also controls the output units

Syntax

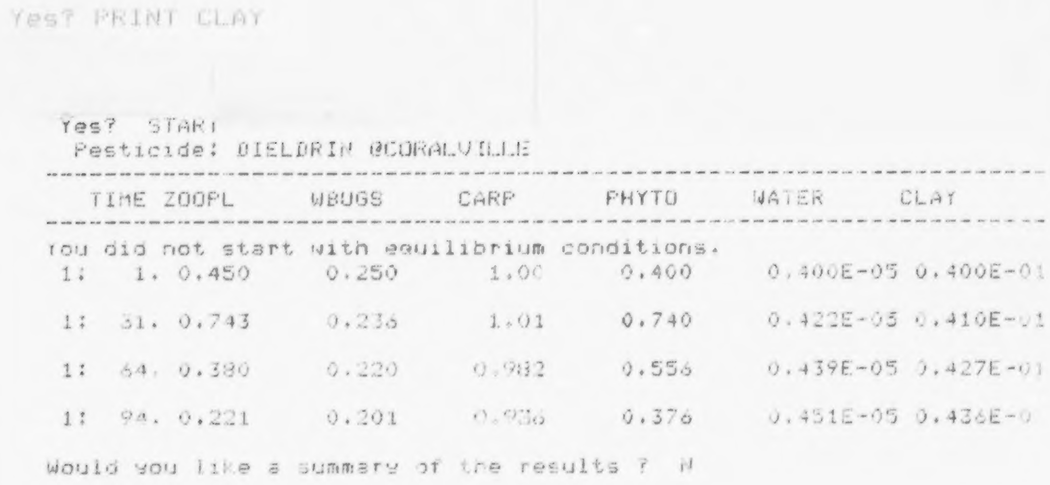
```
PRINT  <item>
```

where

<item> is the name of a state variable or ALL

If "ALL", all state variables are printed; ordinarily state variables 1,2,3,11,13, and 16 are printed.

Example



```
Yes? PRINT CLAY


  Yes?  START
   Pesticide: DIELDRIN @CORALVILLE
---------------------------------------------------------------------
    TIME ZOOPL      WBUGS      CARP       PHYTO      WATER      CLAY
---------------------------------------------------------------------
You did not start with equilibrium conditions.
  1:   1. 0.450      0.250       1.00       0.400      0.400E-05 0.400E-01

  1:  31. 0.743      0.236       1.01       0.740      0.422E-05 0.410E-01

  1:  64. 0.380      0.220      0.982       0.556      0.439E-05 0.427E-01

  1:  94. 0.221      0.201      0.936       0.376      0.451E-05 0.436E-0

Would you like a summary of the results ?  N
```

DEBUG

The DEBUG command causes values to be printed for the indicated processes during the simulation, or it will cause loadings, rates or time to be printed during a display. There are eleven valid process names:

Process Name	Meaning	State Variables Affected
BTRA	Biological transformation	1-12
CONS	Consumption	1-12,14-16
GILS	Gill Sorption	1-13
HYDR	Hydrolysis	13-16
MMET	Microbial Metabolism	14-16
MORT	Mortality	1-12,15
OXID	Oxidation	13-16
PHOT	Photolysis	13-16
SOLU	Solution	13,15
SORP	Sorption	1-16
VOLA	Volatilization	13-14

This command is especially useful for diagnostic purposes; it has the potential for generating large amounts of output!

Syntax

```
DEBUG <pname>[,<pname>...]
```

where

<pname> is the name of a process

```
DEBUG <n>[,<n>...]
```

where

<n> is L for loadings, R for rates, or T for time

Example

```
 Yes?  DEBUG GILS
 Yes?  START
  Pesticide: DIELDRIN @CORALVILLE
-------------------------------------------------------------------------------
   TIME ZOOPL      WBUGS      CARP       PHYTO      WATER      CLAY
-------------------------------------------------------------------------------
You did not start with equilibrium conditions.
 1:   1. 0.450      0.250       1.00       0.400      0.400E-05 0.400E-01


GILSRP:
   0.1029253028E-14    0.0                    -0.3319572265E-12   -0.6329556562E-12
  -0.1156394316E-12   -0.2176511128E-13    0.1187643191E-13    0.0
   0.0                 0.0                 0.1089410680E-11
WCIRC :
   0.3409434668E-13    0.5728111128E-14    0.5101936235E-11    0.6645307568E-11
   0.3394711595E-11    0.2115475330E-11    0.7028356846E-12    0.0
   0.0                 0.0
```

```
BCIRC :
   0.6970726080E-13     0.1172730880E-14     0.3438615614E-08     0.5893749488E-08
   0.1545608530E-08     0.6083629156E-09     0.6733071045E-10     0.0
   0.0                  0.0
DIR   :
   0.7260576688E-11     0.1230369973E-11    -0.2341699501E-08    -0.4465007919E-08
```

TABULATE

Assuming a simulation has already been performed, this command will print out a table of results, with the header and without any debugging and blank lines. This is especially useful if you have debugged some processes, run a simulation, and want uncluttered output.

<u>Syntax</u>

TABULATE

<u>Example</u>

```
 Yes?  TABULATE
DIELDRIN @CORALVILLE
--------------------------------------------------------------------------------
   TIME ZOOPL      WBUGS      CARP       PHYTO      WATER      CLAY
--------------------------------------------------------------------------------
 1:    1. 0.450      0.250       1.00       0.400      0.400E-05 0.400E-01
 1:   31. 0.743      0.236       1.01       0.740      0.422E-05 0.410E-01
 1:   64. 0.380      0.220      0.982       0.556      0.439E-05 0.427E-01
 1:   94. 0.221      0.201      0.936       0.376      0.451E-05 0.436E-01
 Yes?
```

PLOT

This command assumes that a simulation has been done already (there should be some data in files attached to I/O units 2 and 3) and plots the simulation results for the named state variable. XYPLOT subroutine can be modified to suit the user; it takes 3 arguments: an X vector, a Y vector, and the number of points. The state-variable name entered must match one of the heading titles for a simulation.

PLOT normally provides printer plots; however, if at the beginning of a run the question "Are you on a graphics device?"

was answered "Yes", it assumes a configuration similar to that in the Center for Ecological Modeling: a DEC VT55 and an HP722 plotter with proprietary software. The XYPLTA subroutine is used for the HP plotter; it is included as an example of how device-dependent calls can be used.

Syntax

```
PLOT <SVname>
```

where

<SVname> is the name of a state variable; it must match one of the heading titles for the simulation

Example

```
Yes?  PLOT PHYTO
      147.00
  297.00

             --------------------------------------------------------------
 0.44478     :*                                                           :
 0.43217     :                                                            :
 0.41956     :                                                            :
 0.40695     :                                                            :
 0.39434     :                                                            :
 0.38173     : *                                                          :
 0.36913     :                                                            :
 0.35652     :                                                            :
 0.34391     :   *                                                        :
 0.33130     :                                                            :
 0.31869     :     *                                                      :
 0.30609     :                                                            :
 0.29348     :                                                            :
 0.28087     :       *                                                    :
 0.26826     :                                                            :
 0.25565     :         *                                                  :
 0.24305     :                                                            :
 0.23044     :           *                                                :
 0.21783     :             *                                              :
 0.20522     :               *                                            :
 0.19261     :                 *                                          :
 0.18000     :                   *                                        :
 0.16740     :                     *                                      :
 0.15479     :                       *                                    :
 0.14218     :                         * *                                :
 0.12957     :                             * *                            :
 0.11696     :                                 * *                        :
 0.10436     :                                     * *                    :
 0.91747E-01 :                                         * * *              :
 0.79139E-01 :                                               * * * * * * *:
             --------------------------------------------------------------

      147.00
  297.00
Yes?
```

DISPLAY

This will cause a process (see DEBUG) to be plotted as a function of an independent variable, one of the driving variables denoted by a number:

No.	Driving Variable
1-16	carrier compartment
17	temperature
18	windspeed
19	pH
20	dissolved oxygen
21-36	toxic organic matter in carrier 1-1C
37	solar radiation

The plotting is device-dependent (see PLOT). On a CRT, such as the DEC VT55, it plots a well defined profile. The response curves used in the process documentation (SECTION 2) were obtained using this command with an HP plotter. DISPLAY uses the LOOK subroutine and either the XYPLOT subroutine or the XYPLTA subroutine; these can be modified for different devices.

Syntax

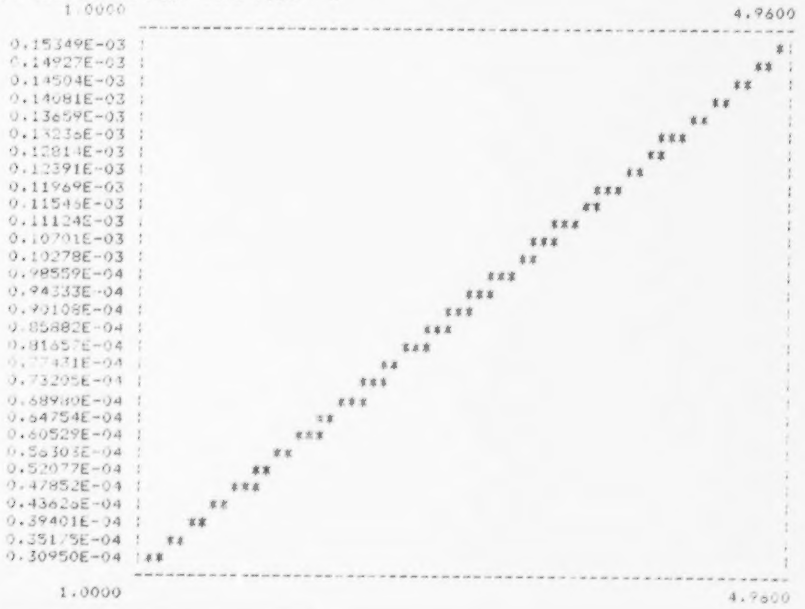
DISPLAY <Pname>

where

<Pname> is a process

Example

```
Yes? DISPLAY VOLA
Which state variable number is to be used ?13
Which loading is to be varied (loading number)?18
Enter the min+max values for the loading : 1,5
Do you want a half-life plot ? N
```



```
Yes? DISPLAY VULA
Which state variable number is to be used ?13
Which loading is to be varied (loading number)?18
Enter the min,max values for the loadings : 1,5
Do you want a half-life plot ? Y
      1.0000                                                         4.9600
             --------------------------------------------------------------
  22391.     :*
  21775.     :                                                            :
  21158.     :*                                                           :
  20542.     : *                                                          :
  19926.     : *                                                          :
  19309.     :                                                            :
  18693.     :  *                                                         :
  18076.     :  *                                                         :
  17460.     :   **                                                       :
  16843.     :    *                                                       :
  16227.     :     *                                                      :
  15611.     :     *                                                      :
  14994.     :      **                                                    :
  14378.     :       *                                                    :
  13761.     :        *                                                   :
  13145.     :         **                                                 :
  12528.     :          **                                                :
  11912.     :           **                                               :
  11296.     :             **                                             :
  10679.     :              ***                                           :
  10063.     :                **                                          :
  9446.3     :                  ***                                       :
  8829.9     :                    ***                                     :
  8213.5     :                       ***                                  :
  7597.0     :                          ***                               :
  6980.6     :                             ****                           :
  6364.2     :                                 ****                       :
  5747.8     :                                     ******                 :
  5131.3     :                                           ********         :
  4514.9     :                                                  **********:
             --------------------------------------------------------------
     1.0000                                                         4.9600
```

DUMP

This command is intended for use in model development and should not be used by the casual user.

DUMP allows the user to look at an entire common block. It accepts as an argument the number of the common block to be printed:

Name	No.	Description
MISC	0	character parameters
RPARMS	1	real parameters
DEBUG	2	logical parameters
TIME	3	integer parameters
DRIVER	4	loadings

Caution: blocks 1 and 4 will usually generate reams of output!

Syntax

```
    DUMP <n> [ n ...]
  where
    <n> is the number of the common block
```

Example

```
    Yes?  DUMP 3
```

```
Parameter dump:
--------- ----

NUMLD :
    20         2         4         4         4         0         0         0         0         0
    20         0         0         0         3         2        20        30        20         6
     0         0         0         0         0         0         0         0         0         0
     0         0         0         0         0         0        24     18772

STEP  :
     5

SWITCH:
    24

IFIRST:
   142

ILAST :
   147
```

HELP

This command provides limited on-line assistance in running the model. It is totally query-oriented and is self-explanatory. However, it is intended to be used as a refresher and not as a substitute for this documentation.

Syntax

    HELP

Example

```
Yes?  HELP

This is the place to be...
Enter a period to get back to command mode.
 What topic do you wish information on?  HELP
 3 line(s) labelled Topics follow.
 Continue? (Yes or No) YES
Legal topics are:  COMMANDS, DEBUG, DISPLAY, DUMP, EDIT,
 HELP INSTALL, LOADINGS, PLOT, PRINT, PROCESSES, QUIT,
 REMOVE, START, TABULATE
 What topic do you wish information on? REMOVE
 3 line(s) labelled Meaning    follow.
 Continue? (Yes or No) Y
   This command allows the user to eliminate a process from
 the simulation.  It can be used to debug nasty processes,
 or to see what the system does if a process is inhibited.
 3 line(s) labelled Syntax    follow.
```

```
Continue? (Yes or No) Y
  The syntax of this command is:
        REMOVE <PROCNAME>
where <PROCNAME> is a process name.
1 line(s) labelled Example   follow.
Continue?  (Yes or No) Y
   REMOVE CONSUM removes consumption from the model.
What topic do you wish information on.
```

QUIT

This command terminates the program and returns control to the operating system.

<u>Syntax</u>

```
QUIT
```

<u>Example</u>

```
Yes?  QUIT

STOP --
```

SECTION 6

PROGRAMMER'S GUIDE

INTRODUCTION

This manual is a guide in bringing up PEST at a particular installation. It is intended to offer the programmer an understanding of the inner structure and rationale of PEST. PEST was written in what we believe to be a structured and modular fashion. This design allows a considerable amount of tampering without a comparable number of nasty side-effects. Thus, any user seeing fit to change a process may do so without much grief. If you find any inadequacies, such as poor commenting in a portion of code or spaghetti code, please use the Software Report Form in the back of this report.

The pesticide model is written in FORTRAN IV, using reasonably standard features. Any system dependencies are hopefully confined to the SPOO subroutine, thus making it easy for the programmer at a particular site to add any system-dependent features (e.g., file openings, program profiling or timing, time of day printout, etc.) according to his sense of aesthetics.

The adage "Small is Beautiful" applies to many of the components in PEST. We have tried to keep the amount of code per subroutine down to a minimum. This hopefully insures easy reading and understanding.

FILE UNITS

PEST uses the following units for I/O:

1	Parameter index file
2	Rates of change of concentration
3	Concentrations
4	Scratch file for conversions
5	User input (terminal)
6	User output (terminal)
8	Help file
9	Parameter file (data)

Files 1 and 8 are text files which are on your distribution tape. File 9 appears on the tape in alphanumeric form and must be converted into an unformatted file before use. See the section "Building a Model" for a description of how to get the parameter file converted.

The parameter index is used by the parameter editor, and each line of this file is in (A1, 6A1, 4I6) format. The first column of this file is reserved for an end-of-file marker. The next six characters are the names of editable parameters. The four integer fields are the common block number to which the parameter belongs, the row and column sizes of the variable (>1 means it is an array), and the location of the parameter in its common block, respectively.

Files 2 and 3 record the results of a simulation in unformatted form for later use by the TAB and PLOT commands, or any external routines the user may have. The first record of these files is the pesticide name, as entered into the parameter PEST; the rest of the records represent values at a particular time during the simulation. Using unformatted FORTRAN I/O they contain the simulation time as the first word, and the next 16 words are the values (rates or concentrations) for each of the state variables. On some machines these values will require two or more words, since the term "word" is somewhat arbitrary to begin with (specifically, DEC computers will use two words for these values, that being the size of their real number). Thus, it should be easy to save simulations for later examination merely by saving those files which were attached to FORTRAN units 2 and 3. You should have enough information now to be able to retrieve the data in these files for printing and plotting, if you so desire. Note that there are a varying number of records in each file, depending on the values of the STEP and TLAST parameters, so that any external routines you write for these data should use the "END=" construct.

File 4 is a scratch file used by the subroutine TRVAL to perform translations from alphanumeric to other modes using FORTRAN I/O. It is not an elegant way of doing things, and will probably be replaced in the future.

Files 5 and 6 should be associated with the user's terminal.

File 8 is the help file. It is in the following format:

```
●
●
●
topic name
xl<subtopic name 1>
●
xl lines of text
●
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD; BEGIN SECTIONS HERE

```
x2<subtopic name 2>
●
x2 lines of text
●
●
xn<subtopic name n>
followed by xn lines of text
topic name
●
●
●
```

In other words, the file starts with a topic name. The topic is divided into subtopics by putting lines in which contain a number-of-lines-to-follow (i2 format), and the subtopic name. Then comes the specified number of lines, followed by another subtopic name, or a topic name, which indicates the end of the previous topic.

File 9 is a sequential access file consisting of 5 unformatted records, one for each parameter common block, whose descriptions appear in the next section. Note that if you wish to change any of these unit numbers you should change the appropriate initializations in the block data which appears in p.main...ftn.

COMMON BLOCKS

The following common blocks are all declared in the main program.

DEBUG - contains the LOGICAL parameters for the model, and is read in by subroutine PARMIO. These parameters control ice cover and debugging of processes.

EATIT - information from the CONSUM subroutine for use by other processes. Contains consumption rates, respiration rates, and grazing rates of various carriers.

DEVICE - contains one logical variable which, if true, indicates that the user wants to produce plots on a graphics device.

DRIVER - is a parameter common block read in by subroutine PARMIO. It contains the values of the driving variables, along with their times of occurrence, if any.

PFLAGS - controls the printing of compartment (carrier) pesticide concentrations during simulations. Each element of the array in PFLAGS is a logical variable corresponding to a particular state variable. If its value is false, the

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

corresponding state variable is not reported on during a simulation.

PLOADS - in this common block is stored the array of loadings for the previous time step.

LODING - contains the loadings for the current time step.

MISC - contains the alphanumeric parameters, specifically the titles for each of the state variables, and the name of the pesticide.

IOUNIT - contains integers which dictate the I/O units for various purposes.

REMSWS - contains a set of flags which determine if a process has been removed or not.

RPARMS - contains the real parameters for the model, and is read in by PARMIO; these are mostly chemical-specific variables.

SEG - reserved for expansion into multiple segments.

SOLUTN - at any one time this common block contains the concentrations of pesticide in each state variable.

TIME - the integer parameter block, read in by PARMIO. Contains STEP, TFIRST, TLAST, and the numbers of each of the loadings (driving variables).

BUILDING A MODEL

Each parameter file actually defines a different model, since it contains chemical, environmental, and biological data that change from system to system. Any of the sixteen compartments in PEST can be redefined to represent another carrier by resetting the parameters for that compartment. This makes it easier to model what you want to model, as long as it falls into one of three categories: plant, animal, or non-living.

Your distribution tape should contain a sample parameter file for you to play with, along with source code for PEST, the source code for the parameter conversion program, the parameter index file, the help text file, and the documentation. The tape itself is a 1600 BPI, EBCDIC tape formatted into fixed blocks of 1600 bytes, with 80-byte logical records (FB(1600,80) is the MTS designation), unless otherwise requested. Therefore, if you're not sure of the format, try the above.

The very first file on the tape should contain an index of what is on the tape, and where it is (in the form of an MTS command file, which should be documented well enough to tell you what's going on). As a backup, in case somebody fouled up, you will be sent a copy of that index file along with the tape.

The first thing you should do is get all the files off the distribution tape. Then, obtain the parameter file and prepare it for use by PEST. To do this, perform the following steps:

1) get the parameter file off the tape.
2) get the parameter conversion routine (CONVRT.FOR).
3) compile and link CONVRT.FOR
4) execute the resulting program with unit 2 assigned to the formatted parameter file, and unit 1 assigned to the new unformatted file.
5) when the program asks "To Tape?", hit the return key.

The information in the new file is now usable by PEST, and this file should be assigned to unit 9.

At this point, you can compile the PEST program (all those files beginning with "P", and ending with ".FTN"). If you get any compiler errors, call (518) 270-6494 or send us the Software Report Form in the back of this report. We are striving to make this program as portable as possible.

You have a choice at this point. The SPOO subroutine is a program designed to make the environment as comfortable as the programmer wishes. We use it to convert all input to upper case, and to assign unit numbers to files, so that the user does not have to. If you don't want the subroutine around, you can delete the call to it which occurs in the main program.

SECTION 7

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EPA-287 (Cin.)
(4-76)

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EPA-287 (Cin.)
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APPENDIX A

Parameters and Loadings used in Simulation of Pond A-7, Dor, Israel

```
  HEADER:
TIME   ZOOPL  WBUGS  CARP   SLCARP GRCARP TILAPI <<7>>  <<8>>  <<9>>
<<0>>  PHYTO  MACRO  WATER  <POM>  POM    CLAY

  PEST  :
PARATHION @A7,ISRAEL

  TITLE1:
ZOOPL

  TITLE2:
WBUGS

  TITLE3:
CARP

  TITLE4:
SLCARP

  TITLE5:
GRCARP

  TITLE6:
TILAPI

  TITLE7:
<<7>>

  TITLE8:
<<8>>

  TITLE9:
<<9>>

  TITLEA:
<<0>>

  TITLEB:
PHYTO

  TITLEC:
MACRO

  TITLED:
WATER

  TITLEE:
<POM>

  TITLEF:
POM
```

```
 TITLEG:
CLAY

 TITLE1:
TIME

 00001 :
 0.200E-01  0.200E-01

 00002 :
 1.00

 AEFAT :
 0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451

 ALPHA :
 0.280E-C2  0.280E-C2  C.260E-02  0.250E-02  0.240E-02  0.230E-02  0.220E-02  0.210E-02  0.200E-02  0.190E-02  0.180E-02  0.152E-02

 BACB  :
 0.200E-02  C.100E-C2  C.500E-02

 BDINT :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 BDSLP :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 BLDC2 :
 0.588E+C4  0.588E+C4  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04

 PMIN  :
 0.150      0.300E-02  C.300E-01  0.300E-01  0.300E-01  0.300E-01  1.00       1.00       1.00       1.00

 BTMAX :
 0.312E-03  0.312E-C3  0.312E-03  0.312E-03  0.312E-03  0.312E-03  0.312E-03  0.312E-03  0.312E-03  0.312E-03  0.312E-03  0.312E-03

 BTTIM :
 8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00

 CMAX  :
 1.00       0.100E-02  C.900E-02  0.900E-02  0.900E-02  0.900E-02  1.00       1.00       1.00       1.00

 CONCEN:
 0.0        0.0        C.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.910E-01  0.0        0.0        0.0

 CSAT  :
 24.0

 CYCLE :
 147.

 D     :
 100.

 DELTA :
 0.100

 E     :
```

EPA-287 (Cin.)
(3-76)

```
0.300      1.00       1.00       1.00       1.00       1.00       -1.00      -1.00      -1.00      -1.00      0.0        1.00
0.0
0.300      0.300      C.300      0.300      0.300      0.300      -1.00      -1.00      -1.00      -1.00      0.0        0.0
0.0
0.300      0.100      1.00       1.00       1.00       1.00       -1.00      -1.00      -1.00      -1.00      0.0        0.0
0.0
0.300      0.100      1.00       1.00       1.00       1.00       -1.00      -1.00      -1.00      -1.00      0.0        0.0
0.0
0.300      0.100      1.00       1.00       1.00       1.00       -1.00      -1.00      -1.00      -1.00      0.0        0.0
0.0
0.300      0.100      1.00       1.00       1.00       1.00       -1.00      -1.00      -1.00      -1.00      0.0        0.0
0.0
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00

 ELAM  :
0.480E+04  0.450E+04  0.425E+04  0.375E+04  0.325E+04  0.275E+04  0.235E+04  0.200E+04  0.160E+04  0.155E+04  0.140E+04  950.

 EN    :
0.167E+05  0.167E+05  0.167E+05  0.150E+05

 EBECF :
0.100E-02

 FATRAT:
0.100E-C7  0.100E-C7  0.300E-03  0.300E-03  0.300E-03  0.300R-03   1.00       1.00       1.00       1.00

 FEDSWT:
 1.00      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 FMAX  :
0.600E-01   1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00

 HA    :
0.0        0.0        0.0        0.0

 HB    :
0.0        0.0        0.0        0.0

 HENRY :
0.6C7E-05

 IIMEAS:
0.300E+14

 KA    :
0.0        0.0        0.0        0.0

 KB    :
0.0        0.0        C.0        0.0

 KBTRAN:
 6.00       6.0C       6.00       6.00       6.00       6.00       6.00       6.00       6.00       6.00       6.00       6.00
```

TYPING GUIDE SHEET

BEGIN FIRST LINE OF TEXT HERE

CENTER OF PAGE

TOP OF IMAGE AREA

DROPPED HEAD: BEGIN SECTION HERE

BEGIN LAST LINE OF TEXT

3/8"

BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS

EPA-287 (Cin.) (4-76)

```
 KCAI  :
0.0        0.0        0.732      0.201E-01

 KDEPTH:
0.200E-01

 KDIFF :
0.457E-05

 KEFF  :
0.0        0.0        0.0        0.0

 KEC   :
0.316E-04

 KEPD  :
 6.00       6.00       6.00       6.00       6.00      0.100

 KEXCR :
0.300      0.300      0.300      0.300      0.300      0.300      1.00       1.00       1.00       1.00

 KH    :
0.0        0.0        0.0        0.0

 KMEAS :
0.0

 KMCRT :
0.500E-04  0.250E-04  0.100E-02  0.100E-02  0.100E-02  0.100E-02  0.0        0.0        0.0        0.0        0.200E-04  0.500E-04

 KC    :
0.302E-02  0.364E-02  0.364E-02  0.364E-02

 KC2   :
0.100      0.0        0.400E-01  0.400E-01  0.400E-01  0.400E-01  0.0        0.0        0.0        0.0

 KCH   :
43.2        43.2       43.2       43.2

 KP    :
0.0        0.0        0.0        0.0

 KPART :
480.        70.0       70.0       6.54

 KPH   :
1.00        1.00       1.00       1.00

 KRESP :
0.250      0.400      0.350      0.350      0.350      0.350      1.00       1.00       1.00       1.00

 KS    :
20.0        20.0       20.0

 KT    :
1.00        1.00       1.00       1.00

 KTEMP :
0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  1.00       1.00       1.00       1.00
```

```
 KTE    :
 1.00       1.00       1.00       1.00

 KTURB  :
 6.00       6.00       6.00       6.00       6.00       6.00

 LIFHIL:
0.200E-01

 METMAX:
 10.0       10.0       10.0

 MKC2   :
0.200E-01  0.200E-01  0.200E-01

 MMGT   :
 2.00       2.00       2.00

 MCLCNT:
 291.

 NUMB   :
0.0

 CCCND :
-1.00      -1.00      C.100      0.200      0.390      -1.00       1.00      0.0        0.900E-02  0.0        0.0        0.0
-1.00      -1.00      0.100      0.200      0.250      -1.00       1.00      0.0        0.900E-02  0.0        0.0        0.0
-1.00      -1.00      -1.00      0.200      0.400      0.600E-01   1.00      0.0        0.900E-02  0.0        0.100      0.0
-1.00      -1.00      -1.00      0.200      0.400       1.00       1.00      0.0        0.900E-02  0.0        0.0        0.0
-1.00      0.600      -1.00      -1.00      0.400       1.00       1.00      0.0         1.00      0.0        0.400E-01  0.336
-1.00      0.100      -1.00      -1.00      0.400       1.00      0.0        0.0         1.00      0.0        0.400E-01  0.336
-1.00      0.100      0.0        -1.00      -1.00       1.00      0.0         1.00       1.00      0.0        0.400E-01  0.336
-1.00      0.100      0.150      -1.00      -1.00       1.00      0.0        0.100E-02   1.00      0.0        0.400E-01  0.336

 PARAMS:
0.302E-02  0.364E-02  0.364E-02  0.364E-02  0.0        0.0        0.0        0.0         43.2       43.2       43.2       43.2
0.0        0.0        0.732      0.201E-01  0.167E+05  0.167E+05  0.167E+05  0.150E+05  0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 1.00       1.00       1.00       1.00      0.607E-05   303.       14.8       96.0       1.00       147.      0.100E-02  0.280E-02
0.280E-02  0.260E-02  0.250E-02  0.240E-02  0.230E-02  0.220E-02  0.210E-02  0.200E-02  0.190E-02  0.180E-02  0.152E-02  0.480E+04
0.450E+04  0.425E+04  0.375E+04  0.325E+04  0.275E+04  0.235E+04  0.200E+04  0.160E+04  0.155E+04  0.140E+04   950.      0.0
0.300E+14   100.      0.170E-03  0.0         7.00      0.100      0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.910E-01  0.0        0.0        0.0         2.00       2.00
 2.00      0.333E-01  0.333E-01  0.333E-01   67.0      0.0        0.0        0.200E-02  0.100E-02  0.500E-02   10.0       10.0
 10.0       20.0       20.0       20.0       6.00       6.00       6.00       6.00       9.00       9.00       9.00       9.00
 1.00       1.00       1.00       1.00       298.       298.       298.       298.      0.100E-01  0.150      0.100      0.100
0.100      0.100      -1.00      -1.00      -1.00      -1.00      0.0        0.250      0.200      0.200      0.200      0.200
-1.00      -1.00      -1.00      -1.00      0.0        0.250E-01  0.0        0.0        0.0        0.0        -1.00      -1.00
-1.00      -1.00      0.0        0.250E-01  0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00
0.0        0.250E-01  C.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      0.0        0.250E-01
0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
0.600      0.100      C.100      0.100      0.100      0.100      -1.00      -1.00      -1.00      -1.00      0.0        0.150
0.200      0.200      0.200      0.200      -1.00      -1.00      -1.00      -1.00      0.390      0.250      0.400      0.400
0.400      0.400      -1.00      -1.00      -1.00      -1.00      0.600E-01   1.00       1.00       1.00       1.00       1.00
 1.00       1.00       1.00       1.00       1.00      0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         1.00      0.100E-02  0.900E-02  0.900E-02  0.900E-02  0.900E-02   1.00       1.00       1.00       1.00
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EPA-287 (Cin.)
(4-76)

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0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0          1.00        1.00
0.400E-01   0.400E-01   0.400E-01   0.0         0.0         0.0         0.0         0.0         0.500       0.0         0.500       0.500
0.500       0.0         0.0         0.0         0.0         0.0         0.451       0.451       0.451       0.451       0.451       0.451
0.451       0.451       0.451       0.451       0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01
0.200E-01   0.200E-01   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04    216.        34.0
 35.0        31.5        34.5        33.5        50.0        50.0        50.0        50.0        50.0        30.0        30.0       0.500E-04
0.250E-04   0.110       0.700E-01   0.400E-01   0.0         0.0         0.0         0.0         0.0         0.200E-04   0.500E-04    8.00
 8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00       0.313E-01
0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01    1.00
 1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00       0.100
0.100       0.100       0.100       0.596E-05    1.00        17.0       0.0          20.0        20.0        20.0        20.0        30.0
 30.0        30.0        30.0        1.00        1.00        1.00        1.00       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
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0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0          266.        630.        90.0        90.0        7.46       0.100E-01   0.100E-01   0.100E-01   0.100E-01
0.100E-01    1.00        1.00        1.00        1.00        1.00       0.300       0.300       0.300       0.300       0.300        1.00
 1.00        1.00        1.00        1.00       0.200       0.200       0.151       0.182       0.147        1.00        1.00        1.00
 1.00        1.00       0.500E-01   0.500E-01   0.250E-01   0.240E-01   0.220E-01    1.00        1.00        1.00        1.00        1.00
0.100E-07   0.100E-07   0.310E-03  -0.340E-04   0.950E-04   0.300E-03    1.00        1.00        1.00        1.00       0.100E-03   0.100E-03
0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-02   0.100E-02   0.100E-02   0.100E-02
0.100E-02   0.100E-02   0.100E-02   0.100E-02   0.100E-02   0.100E-02   0.400       0.400       0.400       0.400       0.400        1.00
 1.00        1.00        1.00        1.00       0.150       0.300E-02   0.300E-01   0.300E-01   0.300E-01    1.00        1.00        1.00
 1.00        1.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00
 2.00        2.00        2.00        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0
 40.0        40.0        40.0        40.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0
 25.0        25.0        25.0        25.0        25.0       0.316E-04   0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.0
0.0         0.0         0.0         0.0         0.600       0.500E-01   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03
0.500E-03   0.500E-03   0.700       0.500        1.00       0.500       0.500       0.500       UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU
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EPA-287 (Cin.)
(4-76)

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 PCBLD :
0.200       0.200       0.151       0.182       0.147        1.00        1.00        1.00        1.00        1.00

 PCBLW :
 7.00

 PCFAT :
0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.0         0.0         0.0         0.0         0.0

 PCFBL :
 216.

 PFIBOD:
0.500E-01   0.500E-01   0.250E-01   0.240E-01   0.220E-01   0.250E-01    1.00        1.00        1.00        1.00

 PHMAX :
 9.00        9.00        9.00        9.00

 PHMIN :
 6.00        6.00        6.00        6.00

 PRATIC:
 298.       -1.00       0.200       0.0         0.250E-01   -1.00       -1.00       0.0         -1.00       -1.00       -1.00       -1.00
0.100E-01   -1.00       -1.00       0.0         0.0         0.0         -1.00       -1.00       -1.00       -1.00       -1.00       -1.00
0.150       -1.00       -1.00       0.0         0.0         0.250E-01   -1.00       -1.00       -1.00       -1.00       -1.00       -1.00
0.100       0.0         -1.00       -1.00       0.0         0.0         0.0         -1.00       -1.00       -1.00       -1.00       -1.00
0.100       0.250       -1.00       -1.00       0.0         0.0         0.250E-01   -1.00       -1.00       -1.00       -1.00       -1.00
0.100       0.200       0.0         -1.00       -1.00       0.0         0.0         -1.00       -1.00       -1.00       -1.00       -1.00
0.100       0.200       0.250E-01   -1.00       -1.00       0.0         0.0         -1.00       -1.00       -1.00       -1.00       -1.00
-1.00       0.200       0.0         0.0         -1.00       -1.00       0.0         -1.00       -1.00       -1.00       -1.00       -1.00

 PSIA  :
0.170E-03

 PSIB  :
0.0

 C     :
0.400       0.400       0.400       0.400       0.400       0.400        1.00        1.00        1.00        1.00

 Q10   :
 2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00
 2.00

 CT    :
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0

 RAD   :
0.0         0.0         0.0         0.0

 RADIUS:
0.0         0.0         0.0          1.00       0.280E-02   0.152E-02   0.155E+04   0.0         0.0         0.333E-01    10.0        9.00
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EPA-287 (Cin.)
(4-76)

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
DROPPED HEAD: BEGIN SECTIONS HERE
CENTER OF PAGE
TOP OF IMAGE AREA
BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUS TRATIONS
3/8"

```
0.0        0.0        0.0         1.00      0.260E-02  0.480E+04  0.140E+04  0.0        0.0        0.333E-01  20.0       9.00
0.0        0.0        0.0        0.607E-05  0.250E-02  0.450E+04   950.      0.0        0.910E-01   67.0      20.0       1.00
0.0        0.0        0.0         303.      0.240E-02  0.425E+04  0.0        0.0        0.0        0.0        20.0       1.00
0.0        0.0        0.0         14.8      0.230E-02  0.375E+04  0.300E+14  0.0        0.0        0.0        6.00       1.00
0.0        0.0        0.0         96.0      0.220E-02  0.325E+04   100.      0.0        0.0        0.200E-02  6.00       1.00
0.0        0.0        0.0         1.00      0.210E-02  0.275E+04  0.170E-03  0.0         2.00      0.100E-02  6.00       298.
0.0        0.0        0.0         147.      0.200E-02  0.235E+04  0.0        0.0         2.00      0.500E-02  6.00       298.
0.0        0.0         1.00      0.100E-02  0.190E-02  0.200E+04   7.00      0.0         2.00       10.0      9.00       298.
0.0        0.0         1.00      0.280E-02  0.180E-02  0.160E+04  0.100      0.0        0.333E-01   10.0      9.00       298.

 RMAX  :
0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01

 SAFEA :
0.200      0.500E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.300      0.500E-01
 1.00      0.100      C.100      0.900

 SHAPE :
0.607E-05  0.250E-02  0.450E+04   950.      0.0        0.910E-01   67.0      20.0       1.00      0.100      0.200      0.0
 303.      0.240E-02  0.425E+04  0.0        0.0        0.0        0.0        20.0       1.00      0.100      0.200      0.0
 14.8      0.230E-02  C.375E+04  0.300E+14  0.0        0.0        0.0        6.00       1.00      0.100      0.200      0.0
 96.0      0.220E-02  0.325E+04   100.      0.0        0.0        0.200E-02  6.00       1.00      0.100      0.200      0.0
 1.00      0.210E-02  0.275E+04  0.170E-03  0.0         2.00      0.100E-02  6.00       298.      -1.00      -1.00      -1.00
 147.      0.200E-02  C.235E+04  0.0        0.0         2.00      0.500E-02  6.00       298.      -1.00      -1.00      -1.00
0.100E-02  0.190E-02  0.200E+04   7.00      0.0         2.00       10.0      9.00       298.      -1.00      -1.00      -1.00
0.280E-C2  0.180E-02  0.160E+04  0.100      0.0        0.333E-01   10.0      9.00       298.      -1.00      -1.00      -1.00
0.280E-02  0.152E-02  0.155E+04  0.0        0.0        0.333E-01   10.0      9.00      0.100E-01  0.0        0.0        0.0
0.260E-C2  0.480E+C4  C.140E+C4  0.0        0.0        0.333E-01   20.0      9.00      0.150      0.250      0.250E-01  0.250E-01

 STRU  :
0.333E-01  0.333E-01  0.333E-01

 STTOM :
 67.0      0.0        0.0

 TCCND :
0.336      0.451      0.200E-01  0.200E-01  0.0        0.588E+04   35.0      50.0      0.100E-02   8.00       8.00      0.312E-03
0.336      0.451      0.200E-01  0.200E-01  0.0        0.588E+04   31.5      30.0      0.0         8.00       8.00      0.312E-03
0.0        0.451      0.200E-01  0.0        0.0        0.588E+04   34.5      30.0      0.0         8.00       8.00      0.312E-03
0.0        0.451      C.200E-01  0.0        0.0        0.588E+04   33.5      0.500E-04 0.0         8.00      0.312E-03  0.312E-03
0.0        0.451      0.200E-01  0.0        0.588E+04  0.588E+04   50.0      0.250E-04 0.0         8.00      0.312E-03  0.312E-03
0.0        0.451      0.200E-01  0.0        0.588E+04  0.588E+04   50.0      0.100E-02 0.200E-04   8.00      0.312E-03  0.312E-03
0.451      0.451      0.200E-01  0.0        0.588E+04   216.       50.0      0.100E-02 0.500E-04   8.00      0.312E-03  0.312E-03
0.451      0.451      0.200E-01  0.0        0.588E+04   34.0       50.0      0.100E-02  8.00       8.00      0.312E-03   6.00

 TCCPT :
 298.       298.       298.       298.

 TCRIT :
 34.0       35.0       31.5       34.5       33.5       50.0       50.0       50.0       50.0       50.0       30.0       30.0

 TMAX  :
 40.0       40.0       40.0       40.0       40.0       40.0       40.0       40.0       40.0       40.0       40.0       40.0
 40.0

 TOPT  :
 25.0       25.0       25.0       25.0       25.0       25.0       25.0       25.0       25.0       25.0       25.0       25.0
 25.0

 TPMAX :
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PAGE NUMBER
EPA-287 (Cin.)
(4-75)

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 30.0       30.0       30.0       30.0

 TPMIN :
 20.0       20.0       20.0       20.0

 VBEN  :
 96.0

 VFUDGE:
 1.00

 VH2O  :
 14.8

 VTCM  :
 303.

 W     :
0.100E-01  0.0        0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      0.600      0.0
0.390
0.150      0.250      0.250E-01  0.250E-01  0.250E-01  0.250E-01  -1.00      -1.00      -1.00      -1.00      0.100      0.150
0.250
0.100      0.200      0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      0.100      0.200
0.400
0.100      0.200      0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      0.100      0.200
0.400
0.100      0.200      0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      0.100      0.200
0.400
0.100      0.200      0.0        0.0        0.0        0.0        -1.00      -1.00      -1.00      -1.00      0.100      0.200
0.400
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00
-1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00      -1.00
-1.00

 EFFEN :
0.336      0.336      0.336      0.336      0.336      0.336      0.0        0.0        0.0        0.0

 WMIX  :
0.200E-01  0.200E-01  0.200E-01

 DEBUGS:
F F F F F F F F F F
F F F F F F F F F

 DISICE:
F

 DISRAT:
F

 DPROCS:
F F F F F F F F F F
F F F F F F

 DTIME :
```

```
F

  ICE   :
T T T F F F F F F F
F F

  NUMIC :
     15        11         2         2         2         2         0         0         0         0
     14         2         0         0         2         2         3         3         3         3
      0         0         0         0         0         0         0         0         0         0
      0         0         0         0         0         0         3         0

  STEP  :
      1

  SWITCH:
      3

  TFIRST:
     67

  TLAST :
    103

  CLAY  :
 0.500      0.500      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  CLAYT :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0         64.0       79.0       103.      0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  DC2   :
 16.1       16.9        19.0      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  DC2T  :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  FISH1 :
 13.0       30.5       0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  FISH1T:
-87.0       103.       0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  FISH2 :
 5.24       7.50       0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  FISH2T:
```

```
-87.0     103.      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH3 :
0.150     0.500     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH3T:
-87.0     103.      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH4 :
 9.80      2.90     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH4T:
-87.0     103.      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH5 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH5T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH6 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH6T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH7 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH7T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH8 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FISH8T:
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD, BEGIN SECTION HERE
BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

```
0.0      0.0      C.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      C.0      0.0      0.0      0.0

 FCM   :
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      C.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      C.0      0.0      0.0      0.0

 FOMT  :
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0       64.0     79.0     102.    0.0
0.0      0.0      0.0      0.0      0.0      0.0

 LOAD38:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 LDG   :

 LDT   :

 MACBC :
 2.00     2.00    0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 MACRCT:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 PCLAY :
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      C.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 FFISH1:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 PFISH2:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 PFISH3:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 PFISH4:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
0.0      0.0      0.0      0.0      0.0      0.0

 PFISH5:
0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
```

```
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PFISH6:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PFISH7:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PFISH8:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

FFCM  :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PH    :
7.10      8.50      8.55      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PHT   :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PHYTC :
16.8      18.0      8.10      10.5      3.30      3.30      5.10      6.00      12.9      9.90      9.30      5.80
9.00      9.00      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

PHYTCI:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

FMACBC:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

FCM   :
1.50      1.50      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

FCMT  :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       64.0      79.0      103.      0.0
0.0       0.0       0.0       0.0       0.0       0.0

PPHYTC:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
```

```
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FECM  :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 PWATER:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 PWBUGS:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 FZCCEI:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 SCIAR :
 350.      400.      525.     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 TEMP  :
 24.0      19.4      22.3     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 TEMPT :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 WATER :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 WBUGS :
0.180E-02 0.510E-02 0.600E-02 0.600E-03 0.0       0.600E-01 0.0       0.0       0.900E-03 0.300E-03 0.750E-03 0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 WBUGST:
 61.0      64.0      67.0      68.0      74.0      79.0      86.0      89.0      94.0      96.0      103.     0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 WIND  :
 2.32      2.37      2.55     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0

 WINDT :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
```

```
 0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0         0.0

  WIND  :
  2.32        2.37        2.55       0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0         0.0

  WINDT :
 0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0          64.0

  ZCCPI :
 0.451       0.732       0.718        1.00        1.85        1.29        1.27        1.17        1.04       0.803       0.141       0.845E-01
 0.563E-01   0.423E-C1   C.113       0.406E-02   0.900E-02   0.236E-02   0.674E-02   0.214E-02   0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0         0.0

  ZCCFIT:
  61.0        64.0        67.0        68.0        69.0        72.0        74.0        76.0        79.0        81.0        86.0        89.0
  94.0        96.0        103.       0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 0.0         0.0         0.0         0.0         0.0         0.0
& Yes?
```

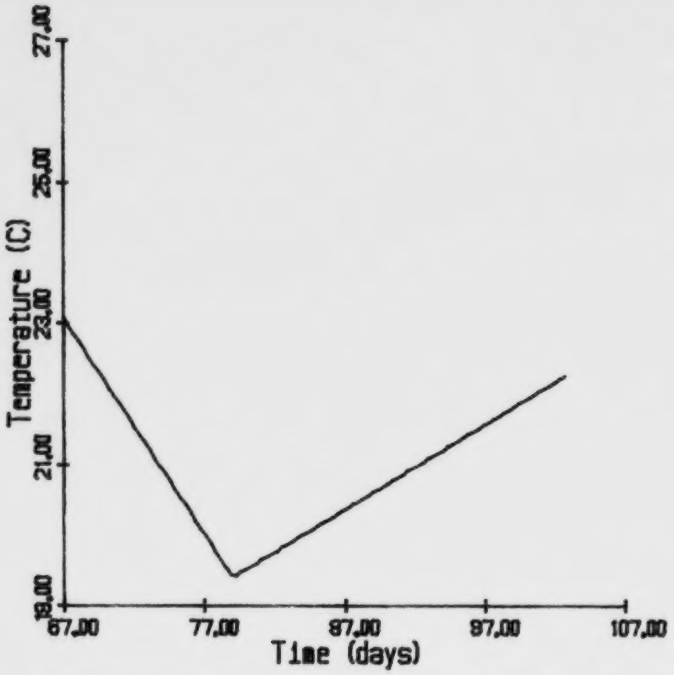

Figure A.1. Temperature loading used in simulation of Pond A-7, Dor, Israel.

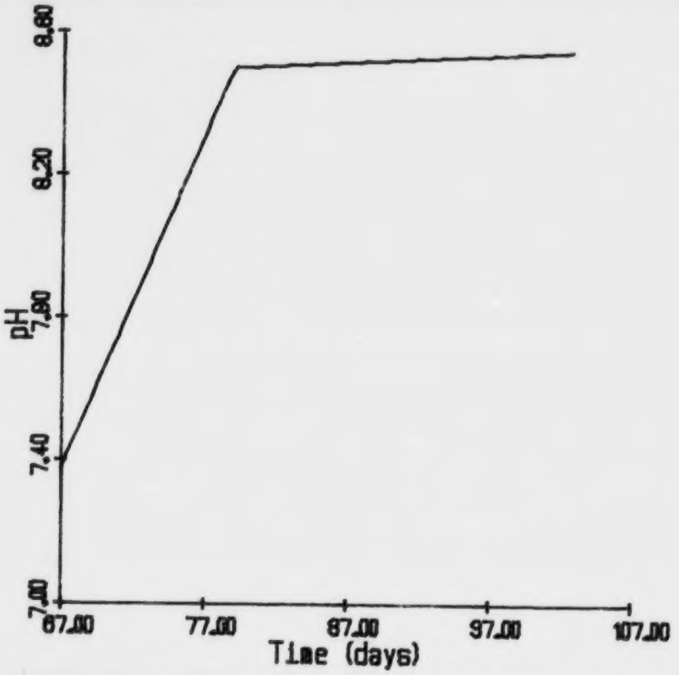

Figure A.2. pH loading used in simulation of Pond A-7, Dor, Israel.

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TYPING GUIDE SHEET
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD, BEGIN SECTIONS HERE

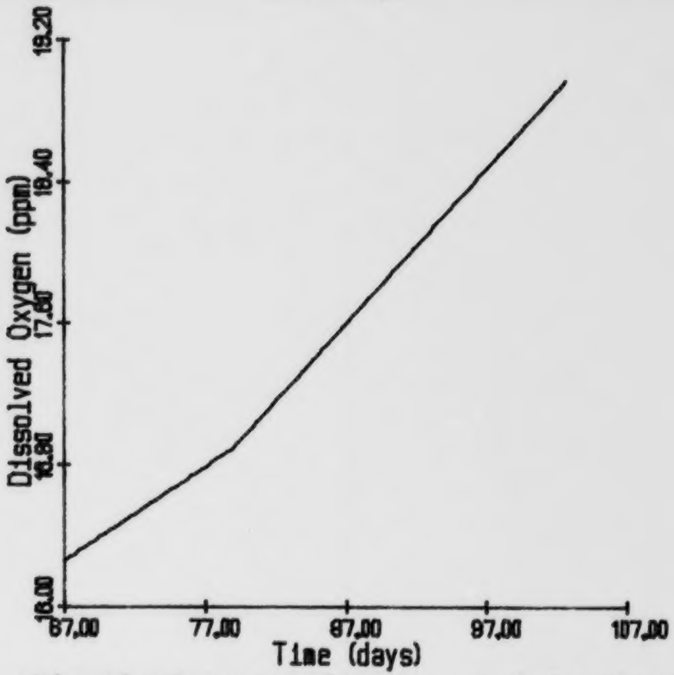

Figure A.3. Dissolved oxygen loading used in simulation of Pond A-7, Dor, Israel.

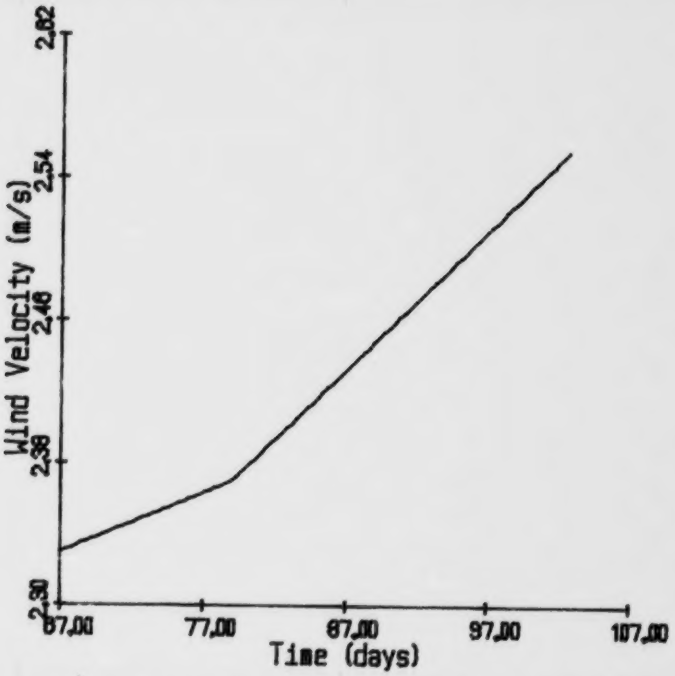

Figure A.4. Wind velocity loading used in simulation of Pond A-7, Dor, Israel.

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PAGE NUMBER

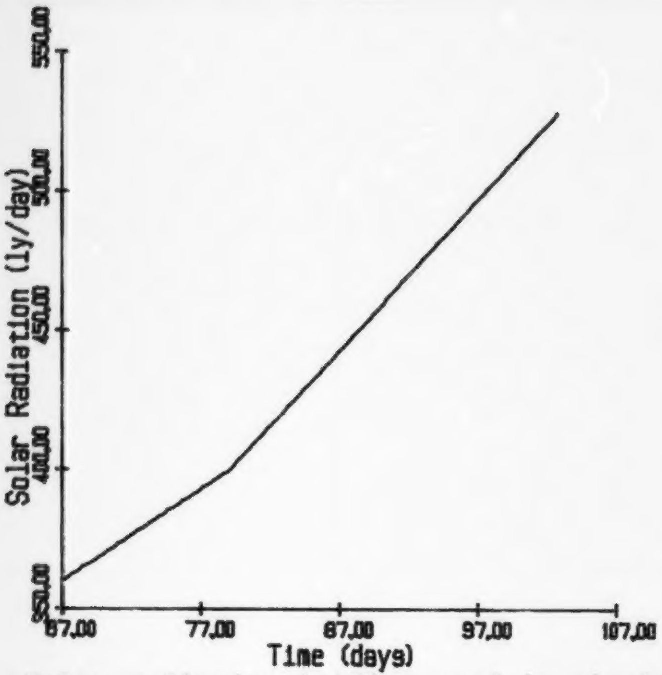

Figure A.5. Solar radiation loading used in simulation of Pond A-7, Dor, Israel.

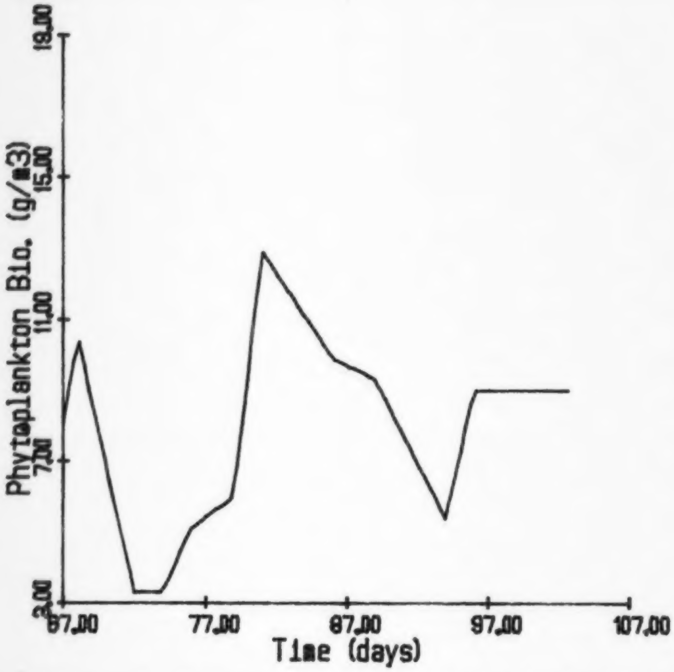

Figure A.6. Phytoplankton biomass used in simulation of Pond A-7, Dor, Israel.

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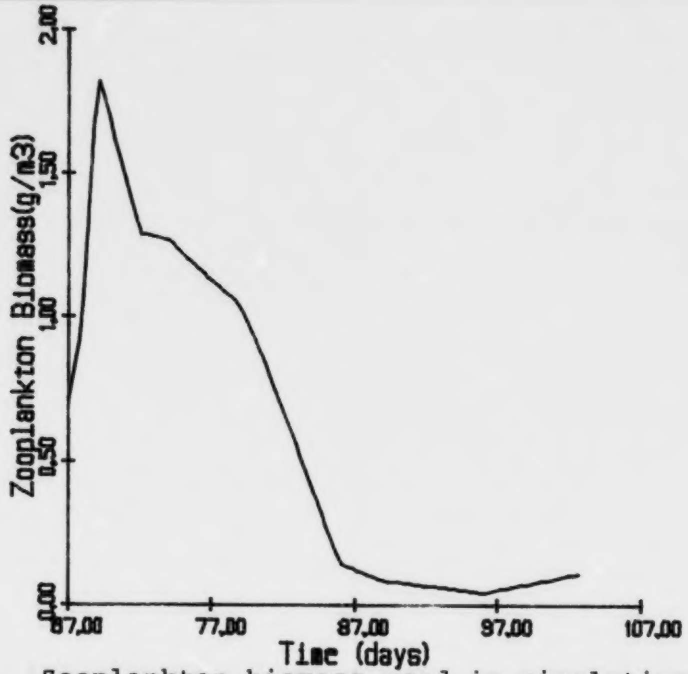

Figure A.7. Zooplankton biomass used in simulation of Pond A-7, Dor, Israel.

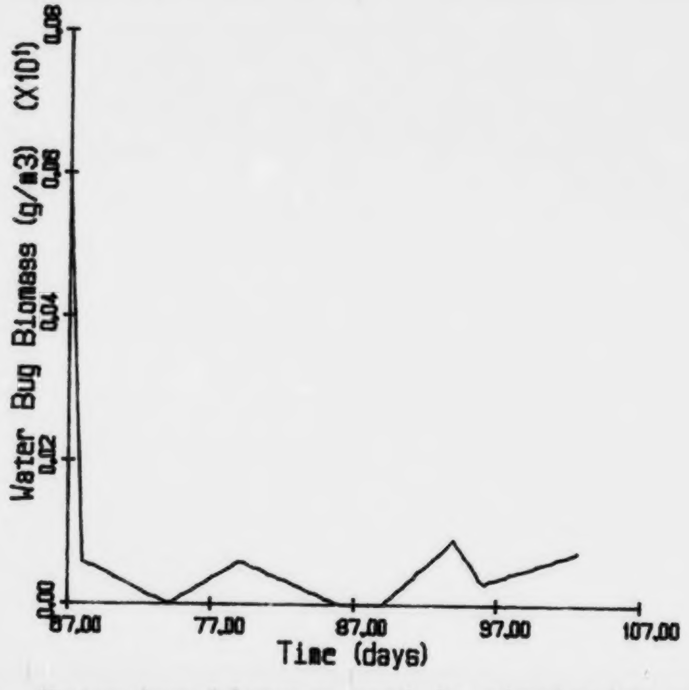

Figure A.8. Water bug biomass used in simulation of Pond A-7, Dor, Israel.

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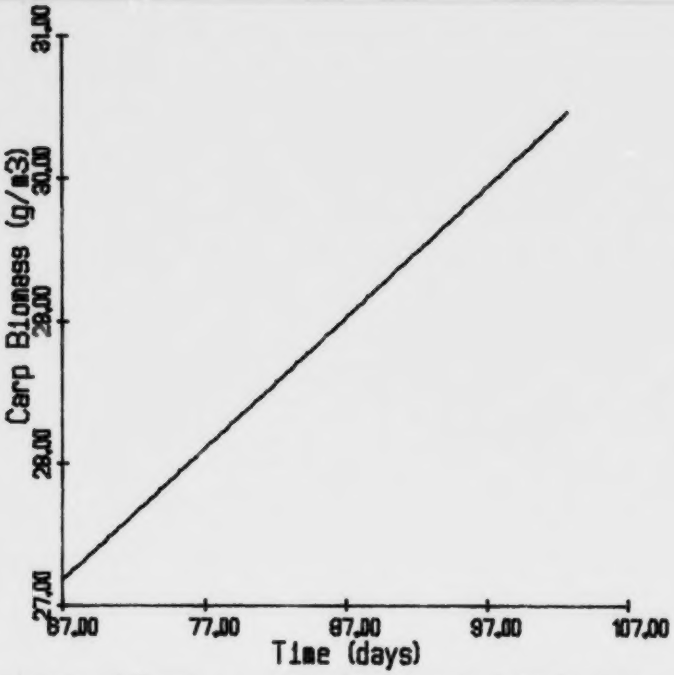

Figure A.9. Carp biomass used in simulation of Pond A-7, Dor, Israel.

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APPENDIX B

Parameters and Loadings Used in Simulation of Treatment-3 Ponds, Columbia, Missouri

```
   HEADER:
 TIME   ZOOPL  WBUGS  BLUGIL LMBASS CHCATF  <<6>>  <<7>>  <<8>>  <<9>>
  <<0>> PHYTO   <MAC> WATER  <PCM>  POM    CLAY

   PEST  :
 PCP  @TRT-3,COLUMBIA

   TITLE1:
 ZOOPL

   TITLE2:
 WBUGS

   TITLE3:
 BLUGIL

   TITLE4:
 LMBASS

   TITLE5:
 CHCATF

   TITLE6:
  <<6>>

   TITLE7:
  <<7>>

   TITLE8:
  <<8>>

   TITLE9:
  <<9>>

   TITLEA:
  <<0>>

   TITLEB:
 PHYTO

   TITLEC:
  <MAC>

   TITLED:
 WATER

   TITLEE:
 <PCM>

   TITLEF:
 POM
 TITLEG:
CLAY

 TITLET:
TIME

 00001 :
 0.200E-01  0.200E-01

 00002 :
 1.00

 AFRAT :
0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451

 ALPHA :
 1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00

 BACB  :
 0.200E-02  0.100E-02  C.500E-02

 BDINT :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 BDSLP :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 BLDC2 :
0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04  0.588E+04

 BMIN  :
0.150      0.300E-02  0.300E-01  0.300E-01  0.300E-01  1.00       1.00       1.00       1.00       1.00

 BTMAX :
0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01  0.313E-01

 BTTIM :
 8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00       8.00

 CMAX  :
 1.00      0.100E-02  C.900E-02  0.900E-02  0.900E-02  1.00       1.00       1.00       1.00       1.00

 CONCEN:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 1.00      0.0        C.0        0.0

 CSAT  :
 17.0

 CYCLE :
 151.

 D     :
 120.

 DELTA :
0.100

 E     :
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0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
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0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600
0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600    0.600
0.600

 ELAM  :
0.252E+04 0.270E+04 0.290E+04 0.326E+04 0.363E+04 0.390E+04 0.433E+04 0.465E+04 0.503E+04 0.510E+04 0.483E+04 0.294E+04

 EN    :
0.970E+05 0.970E+05 0.970E+05 0.970E+05

 ERROR :
0.100E-02

 FATRAT:
0.100E-07 0.100E-07 0.310E-03 -0.340E-04 0.950E-04 0.300E-03  1.00     1.00     1.00     1.00

 FEDSWT:
 1.00     0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0

 FMAX  :
0.600E-01  1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00     1.00

 HA    :
0.0       0.0      0.0      0.0

 HB    :
0.0       0.0      0.0      0.0

 HENRY :
0.310E-06

 XIMEAS:
0.106E+20

 KA    :
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 KB    :
0.0       0.0      0.0      0.0

 KBTRAN:
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 KCAL  :
0.0       0.0       0.0       0.0

 KDEPTH:
0.200E-01

 KDIFF :
0.596E-05

 KEFF  :
0.0       0.0       0.0       0.0

 KEQ   :
0.316E-04

 KEFD  :
 1.00      1.00      1.00      1.00      1.00      0.100

 KEXCR :
0.300     0.300     0.300     0.300     0.300      1.00      1.00      1.00      1.00      1.00

 KH    :
0.113E+05 0.113E+05 0.113E+05 0.113E+05

 KMEAS :
0.0

 KMCRT :
0.500E-04 0.250E-04 0.110     0.700E-01 0.400E-01 0.0       0.0       0.0       0.0       0.0       0.200E-04 0.500E-04

 KC    :
0.583E-02 0.583E-02 0.583E-02 0.583E-02

 KC2   :
 1.00      1.00     C.400E-01 0.400E-01 0.400E-01 0.0       0.0       0.0       0.0       0.0

 KCH   :
 3.34      3.34      3.34      3.34

 KE    :
0.0       0.0       0.0       0.0

 KFART :
 630.      90.0      90.0      7.46

 KFR   :
 1.00      1.00      1.00      1.00

 KRESE :
0.100E-02 0.100E-02 0.100F-02 0.100E-02 0.100E-02 0.100E-02 0.100E-02 0.100E-02 0.100F-02 0.100E-02

 KS    :
 20.0      20.0      20.0

 KT    :
 1.00      1.00      1.00      1.00

 KTEMP :
0.100E-01 0.100E-01 C.100E-01 0.100E-01 0.100E-01 1.00      1.00      1.00      1.00      1.00
```

```
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 KTURE :
 1.00       1.00       1.00       1.00       1.00       1.00

 LIFHIL:
0.200E-01

 METMAX:
 10.0       10.0       10.0

 MKO2  :
0.200E-01  0.200E-01  0.200E-01

 MMGT  :
 2.00       2.00       2.00

 MOLCWT:
 266.

 NUMB  :
0.0

 OCCND :
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0.0        0.0        0.0        0.0        0.800E-01  0.0         1.00      0.0        0.900E-02  0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.190E-01  0.600E-01   1.00      0.0        0.900E-02  0.0         1.00      0.0
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0.0        0.100      0.0        0.0        0.0         1.00      0.0         1.00       1.00      0.0        0.400E-01  0.500
0.0        0.0        0.0        0.0        0.0         1.00      0.0        0.100E-02   1.00      0.0        0.0        0.500

 PARAMS:
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0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
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0.270E+04  0.290E+04  0.326E+04  0.363E+04  0.390E+04  0.433E+04  0.465E+04  0.503E+04  0.510E+04  0.483E+04  0.294E+04  0.0
0.106E+20   120.      0.118E-03  0.0         7.00     0.100      0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0         1.00      0.0        0.0        0.0         2.00       2.00
 2.00      0.100      0.100      0.100       142.       142.       142.     0.200E-02  0.100E-02  0.500E-02   10.0       10.0
 10.0       20.0       20.0       20.0       6.00       6.00       6.00       6.00       9.00       9.00       9.00       9.00
 1.00       1.00       1.00       1.00       298.       298.       298.       298.     0.100E-01  0.760      0.100      0.0
0.100      0.0        0.0        0.0        0.0        0.0        0.0        0.100E-01  0.700      0.100      0.551      0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.270E-01  0.300      0.530E-01  0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.270E-01  0.300      0.530E-01  0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.270E-01  0.300      0.530E-01  0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.900      0.150      0.100      0.0        0.900E-01  0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.900E-01  0.800E-01  0.190E-01  0.0
0.100      0.0        0.0        0.0        0.0        0.0        0.600E-01   1.00       1.00       1.00       1.00       1.00
 1.00       1.00       1.00       1.00       1.00      0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         1.00      0.100E-02  0.900E-02  0.900E-02  0.900E-02   1.00       1.00       1.00       1.00       1.00
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0.500       0.0         0.0         0.0         0.0         0.0         0.451       0.451       0.451       0.451       0.451       0.451
0.451       0.451       0.451       0.451       0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01   0.200E-01
0.200E-01   0.200E-01   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04   0.588E+04    216.        34.0
 35.0        31.5        34.5        33.5        50.0        50.0        50.0        50.0        50.0        30.0        30.0       0.500E-04
0.250E-04   0.110       0.700E-01   0.400E-01   0.0         0.0         0.0         0.0         0.0         0.200E-04   0.500E-04    8.00
 8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00        8.00       0.313E-01
0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01   0.313E-01    1.00
 1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00       0.100
0.100       0.100       0.100       0.596E-05    1.00        17.0       0.0          20.0        20.0        20.0        20.0        30.0
 30.0        30.0        30.0        1.00        1.00        1.00        1.00       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
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0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600       0.600
0.600       0.600       0.600       0.600       0.600       0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0          266.        630.        90.0        90.0        7.46       0.100E-01   0.100E-01   0.100E-01   0.100E-01
0.100E-01    1.00        1.00        1.00        1.00        1.00       0.300       0.300       0.300       0.300       0.300        1.00
 1.00        1.00        1.00        1.00       0.200       0.200       0.151       0.182       0.147        1.00        1.00        1.00
 1.00        1.00       0.500E-01   0.500E-01   0.250E-01   0.240E-01   0.220E-01    1.00        1.00        1.00        1.00        1.00
0.100E-07   0.100E-07   0.310E-03  -0.340E-04   0.950E-04   0.300E-03    1.00        1.00        1.00        1.00       0.100E-03   0.100E-03
0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-02   0.100E-02   0.100E-02   0.100E-02
0.100E-02   0.100E-02   0.100E-02   0.100E-02   0.100E-02   0.100E-02   0.400       0.400       0.400       0.400       0.400        1.00
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 40.0        40.0        40.0        40.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0
 25.0        25.0        25.0        25.0        25.0       0.316E-04   0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.0
0.0         0.0         0.0         0.0         0.600       0.500E-01   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03
0.500E-03   0.500E-03   0.700       0.500        1.00       0.500       0.500       0.500       UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU
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DROPPED HEAD: BEGIN SECTIONS HERE
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BEGIN LAST LINE OF TEXT
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 PCPLD :
 0.200      0.200      0.151      0.182      0.147      1.00       1.00       1.00       1.00       1.00

 PCPLW :
 7.00

 PCFAT :
 0.500E-01  0.500E-01  0.500E-01  0.500E-01  0.500E-01  0.0        0.0        0.0        0.0        0.0

 PCFBL :
 216.

 PFIBCD:
 0.500E-01  0.500E-01  0.250E-01  0.240E-01  0.220E-01  1.00       1.00       1.00       1.00       1.00

 PHMAX :
 9.00       9.00       9.00       9.00

 PHMIN :
 6.00       6.00       6.00       6.00

 PRATIC:
 298.       0.0        0.0        0.300      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.100E-01  0.0        0.0        0.530E-01  0.270E-01  0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.760      0.0        0.0        0.0        0.300      0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.100      0.0        0.0        0.0        0.530E-01  0.270E-01  0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.100E-01  0.0        0.0        0.0        0.300      0.0        0.0        0.0        0.0        0.0        0.0
 0.100      0.700      0.0        0.0        0.0        0.530E-01  0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.100      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.551      0.270E-01  0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 PSIA  :
 0.118E-03

 PSIB  :
 0.0

 Q     :
 0.400      0.400      0.400      0.400      0.400      1.00       1.00       1.00       1.00       1.00

 Q10   :
 2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00
 2.00

 QI    :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 RAD   :
 0.0        0.0        0.0        0.0

 RADIUS:
 0.0        0.0        0.0        1.00       1.00       1.00       0.510E+04  0.0        0.0        0.100      10.0       9.00
```

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0.0         0.0         0.0          1.00       1.00        0.252E+04   0.483E+04   0.0         0.0         0.100       20.0        9.00
0.0         0.0         0.0         0.310E-06   1.00        0.270E+04   0.294E+04   0.0          1.00        142.       20.0        1.00
0.0         0.0         0.0          193.       1.00        0.290E+04   0.0         0.0         0.0          142.       20.0        1.00
0.0         0.0         0.0          14.8       1.00        0.326E+04   0.106E+20   0.0         0.0          142.       6.00        1.00
0.0         0.0         0.0          96.0       1.00        0.363E+04    120.       0.0         0.0         0.200E-02   6.00        1.00
0.0         0.0         0.0          1.00       1.00        0.390E+04   0.118E-03   0.0          2.00       0.100E-02   6.00        298.
0.0         0.0         0.0          151.       1.00        0.433E+04   0.0         0.0          2.00       0.500E-02   6.00        298.
0.0         0.0          1.00       0.100E-02   1.00        0.465E+04    7.00       0.0          2.00        10.0       9.00        298.
0.0         0.0          1.00        1.00       1.00        0.503E+04   0.100       0.0         0.100        10.0       9.00        298.

 BMAX  :
0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03

 SAFEA :
0.600       0.500E-01   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.500E-03   0.700       0.500
 1.00       0.500       0.500       0.500

 SHAPE :
0.310E-06    1.00       0.270E+04   0.294E+04   0.0          1.00        142.       20.0         1.00       0.100       0.700       0.270E-01
 193.        1.00       0.290E+04   0.0         0.0         0.0          142.       20.0         1.00       0.0         0.100       0.300
 14.8        1.00       0.326E+04   0.106E+20   0.0         0.0          142.       6.00         1.00       0.100       0.551       0.530E-01
 96.0        1.00       0.363E+04    120.       0.0         0.0         0.200E-02   6.00         1.00       0.0         0.0         0.0
 1.00        1.00       0.390E+04   0.118E-03   0.0          2.00       0.100E-02   6.00         298.       0.0         0.0         0.0
 151.        1.00       0.433E+04   0.0         0.0          2.00       0.500E-02   6.00         298.       0.0         0.0         0.0
0.100E-02    1.00       0.465E+04    7.00       0.0          2.00        10.0       9.00         298.       0.0         0.0         0.0
 1.00        1.00       0.503E+04   0.100       0.0         0.100        10.0       9.00         298.       0.0         0.0         0.0
 1.00        1.00       0.510E+04   0.0         0.0         0.100        10.0       9.00        0.100E-01   0.0         0.0         0.0
 1.00       0.252E+04   0.483E+04   0.0         0.0         0.100        20.0       9.00        0.760       0.100E-01   0.0         0.0

 STFU  :
0.100       0.100       0.100

 STTOM :
142.        142.        142.

 ICCNC :
0.500       0.451       0.200E-01   0.200E-01   0.0         0.588E+04   35.0        50.0        0.0         8.00        8.00        0.313E-01
0.0         0.451       0.200E-01   0.200E-01   0.0         0.588E+04   31.5        30.0        0.0         8.00        8.00        0.313E-01
0.0         0.451       0.200E-01   0.0         0.0         0.588E+04   34.5        30.0        0.0         8.00        8.00        0.313E-01
0.0         0.451       0.200E-01   0.0         0.0         0.588E+04   33.5        0.500E-04   0.0         8.00        0.313E-01   0.313E-01
0.0         0.451       0.200E-01   0.0         0.588E+04   0.588E+04   50.0        0.250E-04   0.0         8.00        0.313E-01   0.313E-01
0.0         0.451       0.200E-01   0.0         0.588E+04   0.588E+04   50.0        0.110       0.200E-04   8.00        0.313E-01   0.313E-01
0.451       0.451       0.200E-01   0.0         0.588E+04    216.       50.0        0.700E-01   0.500E-04   8.00        0.313E-01   0.313E-01
0.451       0.451       0.200E-01   0.0         0.588E+04    34.0       50.0        0.400E-01    8.00       8.00        0.313E-01    1.00

 ICCPT :
298.        298.        298.        298.

 ICFIT :
34.0        35.0        31.5        34.5        33.5        50.0        50.0        50.0        50.0        50.0        30.0        30.0

 IMAX  :
40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0
40.0

 TCPT  :
25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0
25.0

 IPMAX :
```

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 30.0        30.0        30.0        30.0

 TFMIN :
 20.0        20.0        20.0        20.0

 VREN  :
 96.0

 VFUDGE:
 1.00

 VH2C  :
 14.8

 VTCM  :
 193.

 W     :
0.100E-01  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.900       0.0
0.900E-01
0.760      0.100E-01   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.150       0.0
0.800E-01
0.100      0.700       0.270E-01   0.270E-01   0.270E-01   0.0         0.0         0.0         0.0         0.0         0.100       0.0
0.190E-01
0.0        0.100       0.300       0.300       0.300       0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0
0.100      0.551       0.530E-01   0.530E-01   0.530E-01   0.0         0.0         0.0         0.0         0.0         0.900E-01   0.0
0.100
0.0        0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0
0.0        0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0
0.0        0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0
0.0        0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0
0.0        0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0

  EFFEN :
 0.500      0.0         0.500       0.500       0.500       0.0         0.0         0.0         0.0         0.0

  WMIX  :
 0.200E-01  0.200E-C1   C.200E-01

  DEBUGS:
F F F F F F F F F F
F F F F F F F F F

  DISLCD:
F

  DISRAT:
F

  DFBCCS:
F F F F F F F F F F
F F F F F F

  CTIME :
```

```
F

 ICE   :
F F F F F F F F F F
F F

 NUPLD :
     20        2         4         4         4         0         0         0         0         0
     20        0         0         0         3         2        20        30        20         6
      0        0         0         0         0         0         0         0         0         0
      0        0         0         0         0         0        24         0

 STEP  :
      5

 SWITCH:
     24

 TFIRST:
    142

 TLAST :
    292

 CLAY  :
 1.00        1.00        0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 CLAYT :
 219.        226.        233.        240.        247.        254.        261.        268.        275.        293.        300.        0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         142.        149.        205.        212.
 268.        293.        300.        0.0         0.0         0.0

 DC2   :
 5.00        6.00        6.00        5.70        10.4        9.60        7.50        0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 DC2T  :
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 FISH1 :
 1.55       0.420       0.100E-01    1.20       0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 FISH1T:
 142.        144.        293.        300.       0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 FISH2 :
0.940       0.320       0.100E-01   0.750       0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 FISH2T:
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```
 142.       144.        293.        300.   .  0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH3 :
0.552      0.750E-01   0.100E-01   0.560      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH31:
 142.       144.        293.        300.      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH4 :
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH41:
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH5 :
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH51:
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH6 :
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH61:
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH7 :
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH71:
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
 FISH8 :
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0         0.0         0.0        0.0        0.0
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 162.      167.      172.      177.      182.      187.

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 LDG   :

 LDT   :

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0.0       0.0       0.0       0.0       0.0       0.0

 PCIAY :
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0.0       0.0       0.0       0.0       0.0       0.0

 PFISH2:
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0.0       0.0       0.0       0.0       0.0       0.0

 PFISH3:
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0.0       0.0       0.0       0.0       0.0       0.0

 PFISH4:
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 PFISH5:
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0.0        0.0        C.0        0.0        0.0        0.0

 PFISH8:
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0.0        0.0        0.0        0.0        0.0        0.0

 PFCM  :
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0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PH    :
 7.10       7.70       6.90       7.50       7.20       7.50       7.50       7.50       7.80       7.60       7.60       8.20
 8.20       7.70       7.20       7.50       8.00       8.50       8.30       8.50       7.80      0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PHT   :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PHYTC :
0.333      0.442      0.362      0.424      0.606      0.649      0.483      0.550      0.418      0.571      0.454      0.422
0.445      0.515      0.673      0.280      0.692      0.193      0.127      0.200      0.265      0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PHYTCT:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0         142.       144.       293.       300.
0.0        0.0        0.0        0.0        0.0        0.0

 PMACFC:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 POM   :
0.500       2.50       1.50       1.00      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PCMT  :
 192.       197.       203.       207.       212.       217.       222.       227.       232.       237.       241.       247.
 252.       256.       262.       267.       272.       277.       287.       294.       142.       149.       156.       163.
 170.       177.       184.       198.       205.       212.

 PFHYTC:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
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```
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PECM  :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PWATER:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 PWBUGS:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 FZOOPL:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 SOLAR :
 434.       473.       561.       643.       438.       601.       619.       386.       515.       499.       433.       519.
 500.       465.       407.       418.       307.       378.       371.       370.       274.       340.       267.       288.
0.0        0.0        0.0        0.0        0.0        0.0

 TEMP  :
 24.0       25.0       25.0       25.0       25.3       29.0       30.0       28.3       27.7       27.0       28.0       27.3
 27.0       24.3       25.7       24.0       26.0       21.0       18.0       17.0       20.5      0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 TEMPT :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 WATER :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 WBUGS :
0.200E-02  0.200E-02  0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 WBUGST:
 142.       144.       293.       300.      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 WIND  :
 2.24       2.68       1.79       1.79       5.81       6.71       2.24       3.58       3.13       3.13       3.58      0.894
 3.13       3.13       1.34       1.34       3.13       4.02       1.79       1.79       2.68       2.24       1.79       4.47
 4.47       2.24       4.02       1.79       2.24       3.13

 WINDT :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
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0.0        0.0        0.0        0.0        0.0        0.0

 WIND  :
 2.24       2.68       1.79       1.79       5.81       6.71       2.24       3.58       3.13       3.13       3.58       0.894
 3.13       3.13       1.34       1.34       3.13       4.02       1.79       1.79       2.68       2.24       1.79       4.47
 4.47       2.24       4.02       1.79       2.24       3.13

 WINDT :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0         142.

 ZCCPL :
0.324      0.288E-01  0.216E-01  0.228E-01  0.636E-02  0.518E-01  0.274E-01  0.290E-01  0.306E-01  0.334E-01  0.131E-01  0.366E-01
0.162E-01  0.952E-02  0.642E-02  0.406E-02  0.900E-02  0.236E-02  0.674E-02  0.214E-02  0.163      0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 ZCCFIT:
 142.       149.       156.       163.       170.       177.       184.       198.       205.       212.       219.       226.
 233.       240.       247.       254.       261.       268.       275.       293.       300.       0.0        0.0        0.0
 0.0       0.0        0.0        0.0        0.0        0.0
& Yes?
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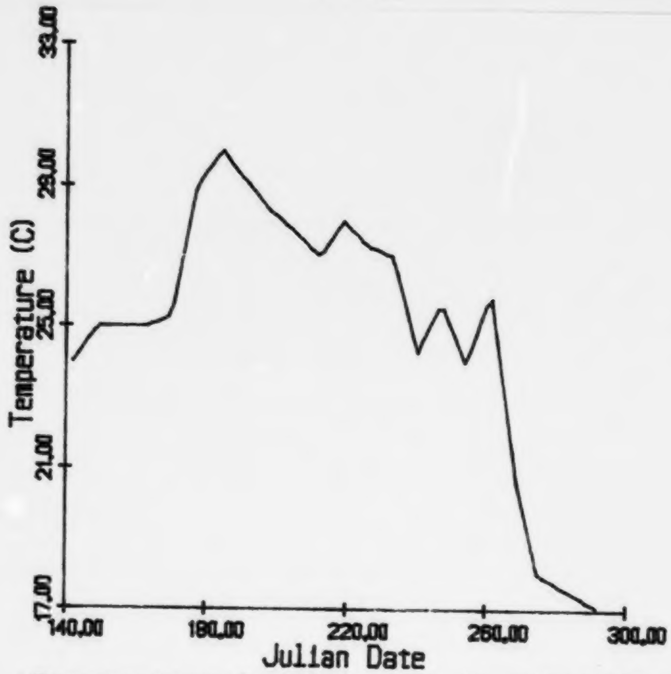

Figure B.1. Temperature loading used in simulation of Treatment-3 ponds, Columbia, Missouri.

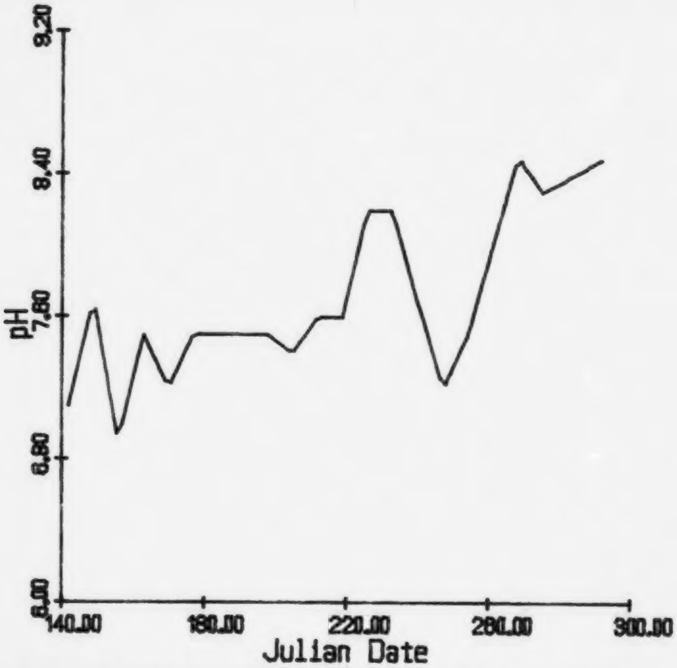

Figure B.2. pH loading used in simulation of Treatment-3 ponds, Columbia, Missouri.

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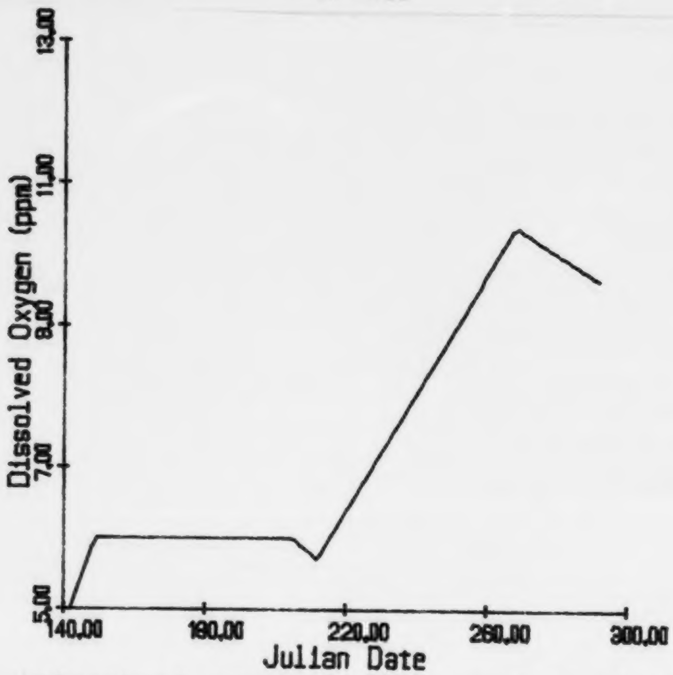

Figure B.3. Dissolved oxygen loading used in simulation of Treatment-3 ponds, Columbia, Missouri.

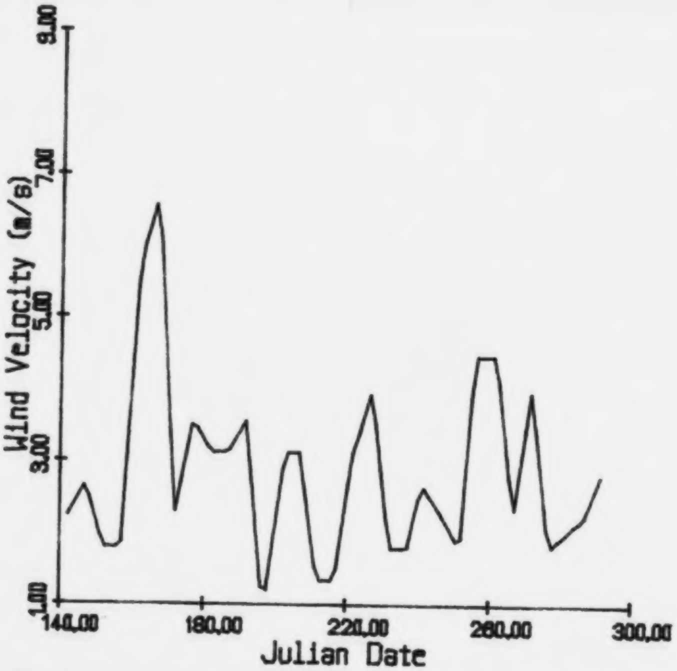

Figure B.4. Wind velocity loading used in simulation of Treatment-3 ponds, Columbia, Missouri.

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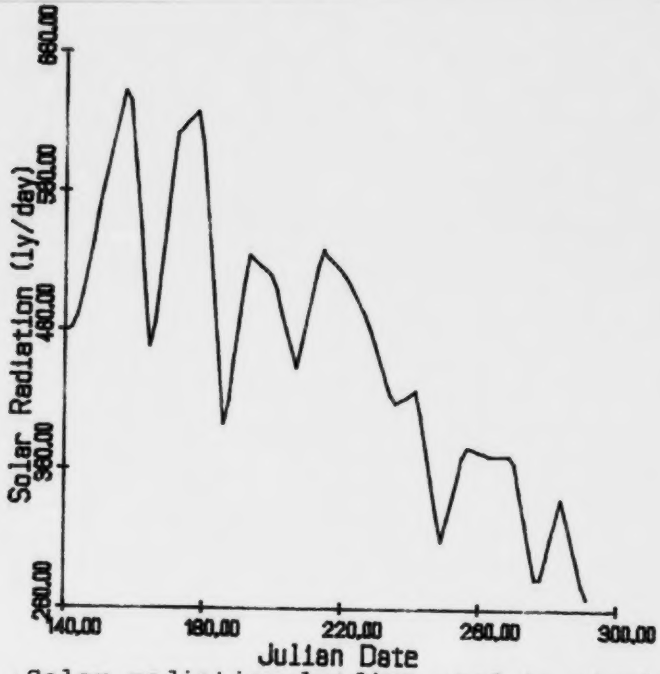

Figure B.5. Solar radiation loading used in simulation of Treatment-3 ponds, Columbia, Missouri.

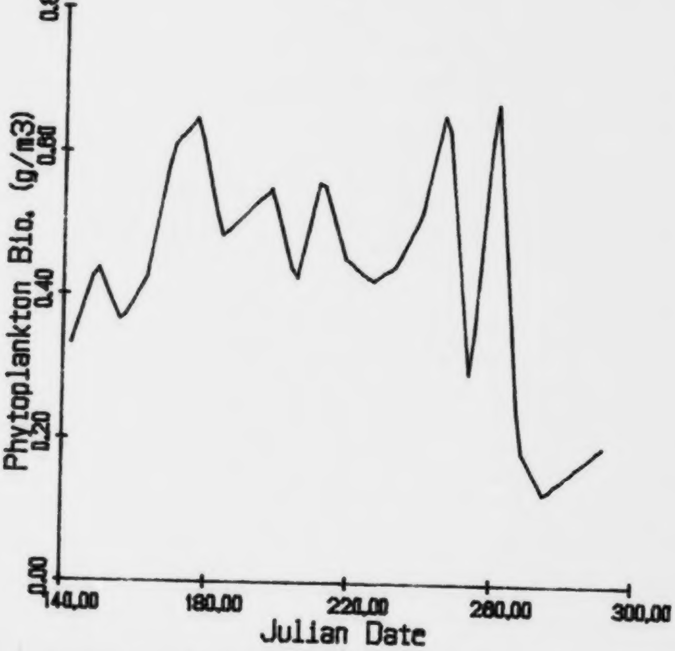

Figure B.6. Phytoplankton biomass used in simulation of Treatment-3 ponds, Columbia, Missouri.

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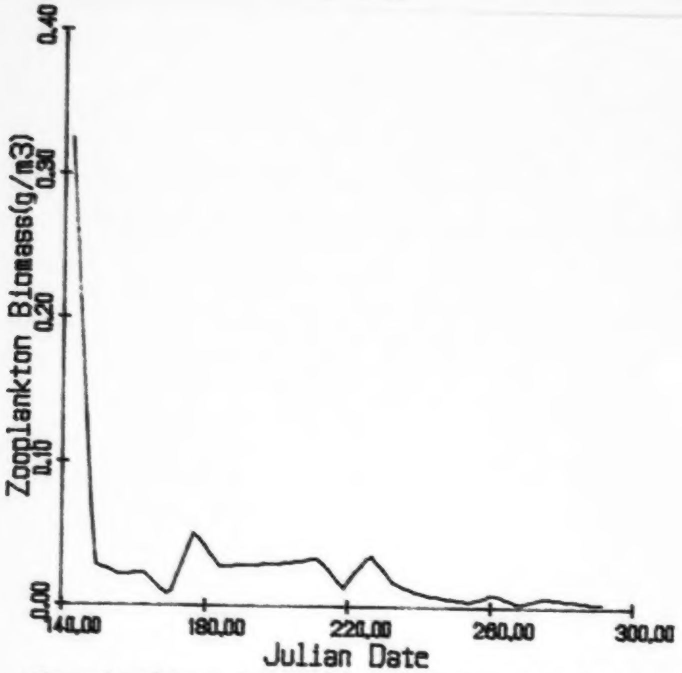

Figure B.7. Zooplankton biomass used in simulation of Treatment-3 ponds, Columbia, Missouri.

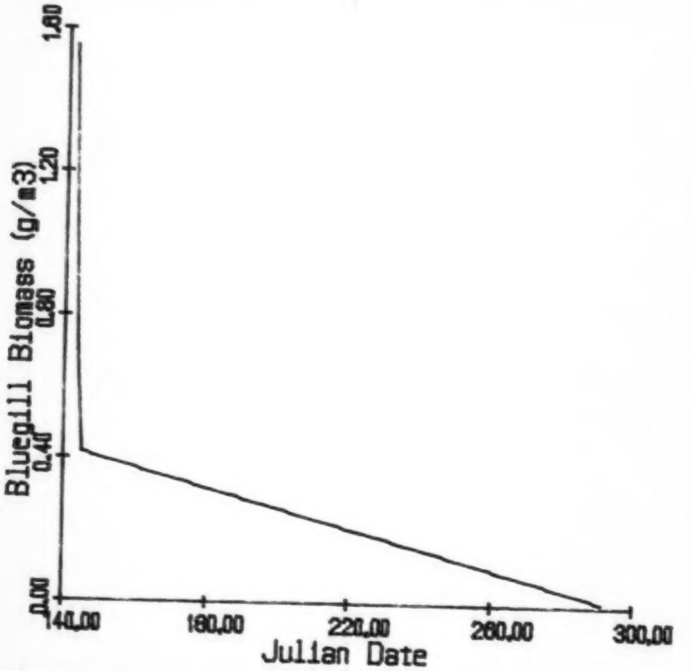

Figure B.8. Bluegill biomass used in simulation of Treatment-3 ponds, Columbia, Missouri.

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APPENDIX C

Loadings used in Simulation of Treatment-2 Ponds, Columbia, Missouri

With the exception of pentachlorophenol-induced mortality, all the parameters are the same as given in Appendix B, as are some of the loadings. Only the loadings that differ from those of Appendix B are illustrated here.

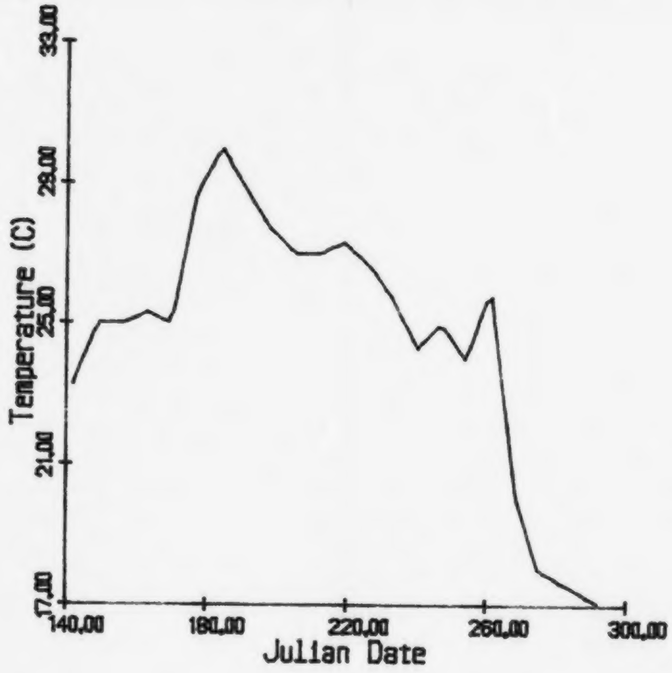

Figure C.1. Temperature loadings used in simulation of Treatment-2 ponds, Columbia, Missouri.

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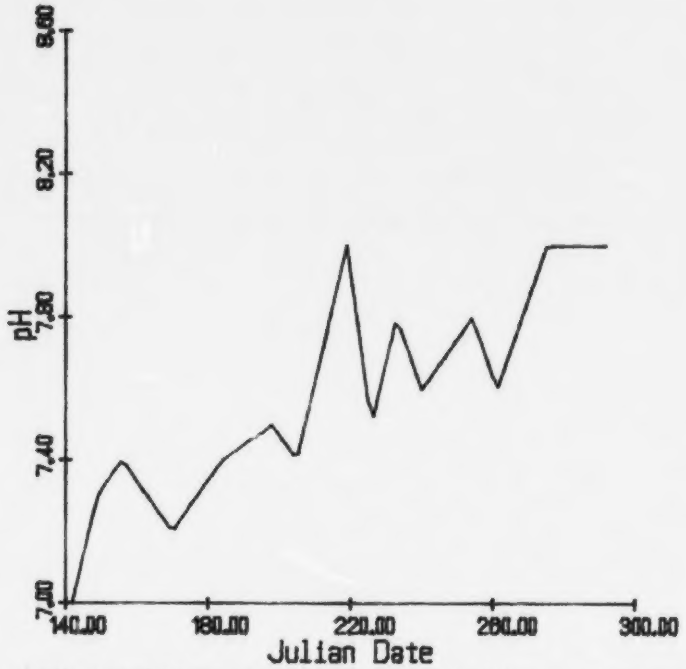

Figure C.2. pH loadings used in simulation of Treatment-2 ponds, Columbia, Missouri.

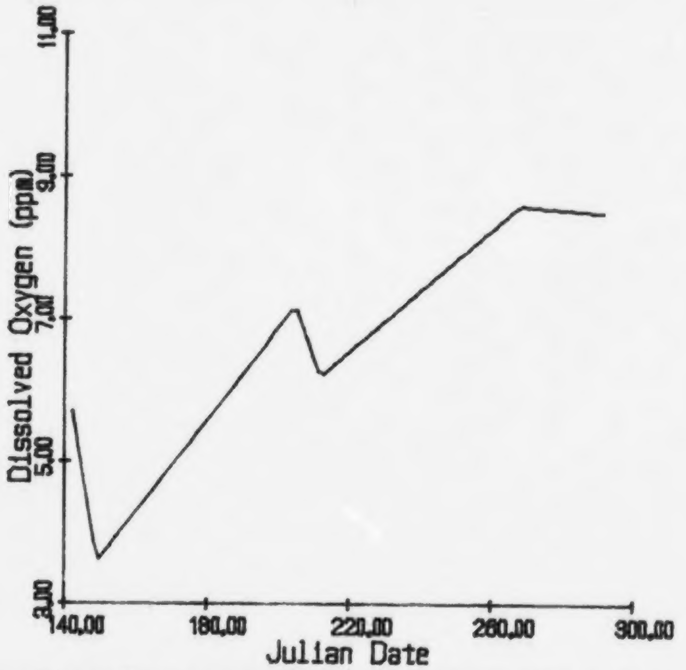

Figure C.3. Dissolved oxygen loadings used in simulation of Treatment-2 ponds, Columbia, Missouri.

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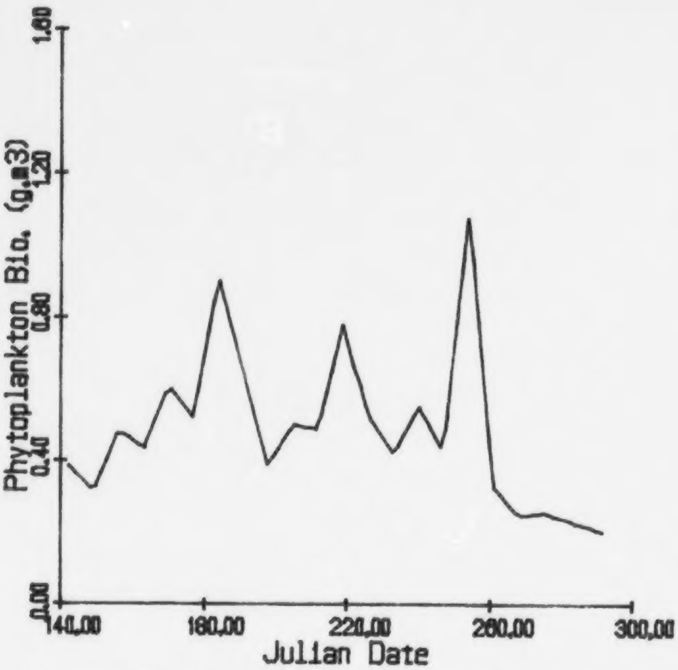

Figure C.4. Phytoplankton biomass used in simulation of Treatment-2 ponds, Columbia, Missouri.

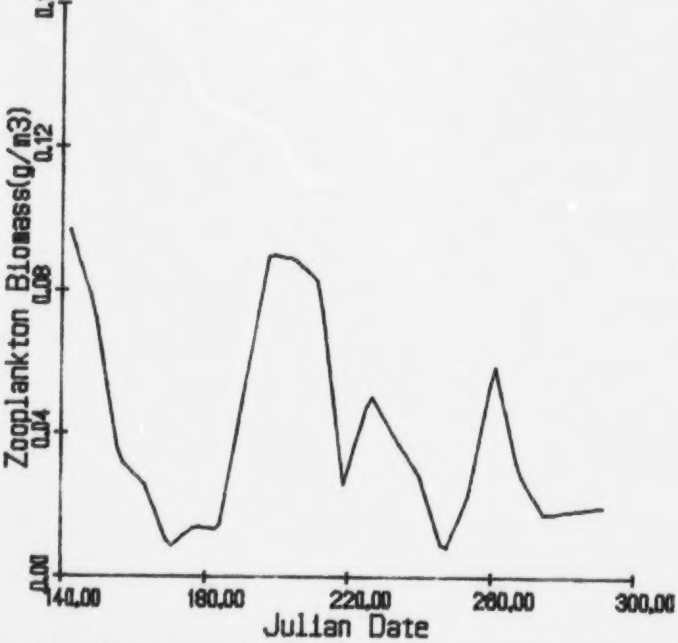

Figure C.5. Zooplankton biomass used in simulation of Treatment-2 ponds, Columbia, Missouri.

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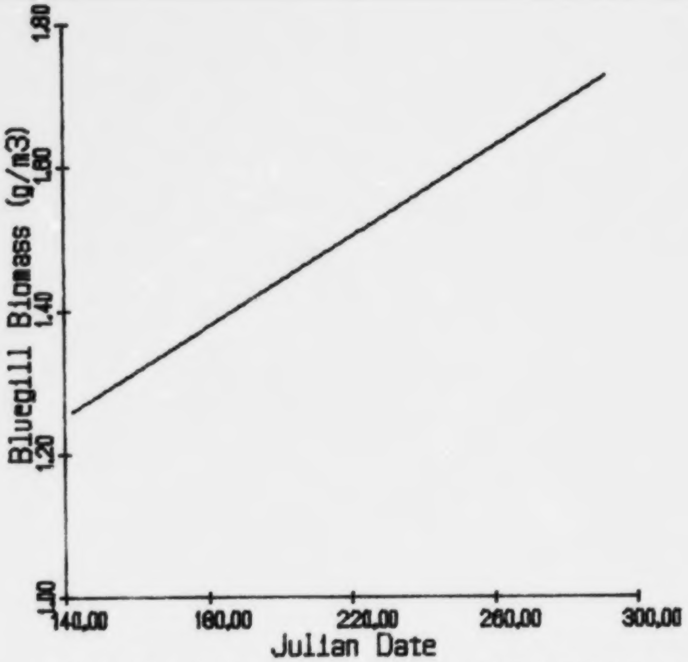

Figure C.6. Bluegill biomass used in simulation of Treatment-2 ponds, Columbia, Missouri.

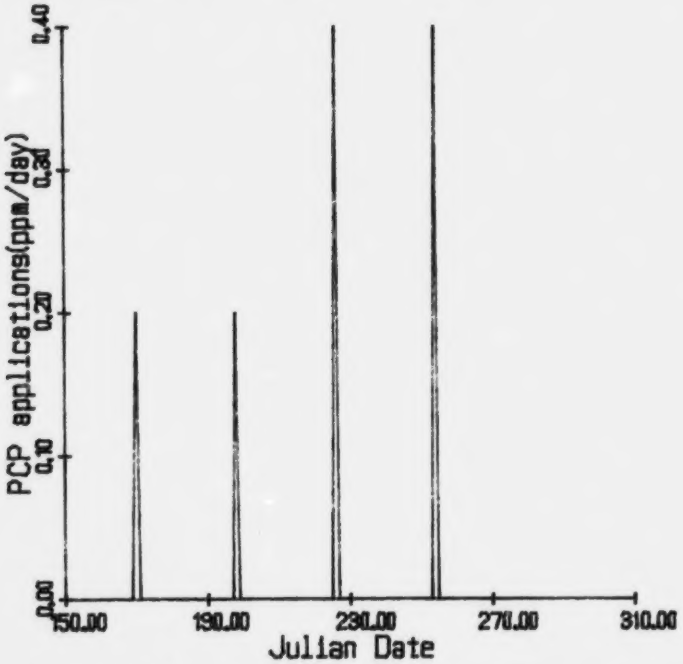

Figure C.7. Pentachlorophenol loadings used in simulation of Treatment-2 ponds, Columbia, Missouri.

APPENDIX D

Parameters and Loadings used in Simulation of Coralville Reservoir, Iowa

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  HEADER:
TTIME  ZOOPL  WBUGS  CARP   BUFALO CHCATF CRAPIE WALEYE <<8>>  <<9>>
<<0>>  PHYTC  MACRC  WATER  <PCM>  PCM    CLAY

  PEST  :
DIELDRIN @CORALVILLE

  TITLE1:
ZOOPL

  TITLE2:
WBUGS

  TITLE3:
CARP

  TITLE4:
BUFALC

  TITLE5:
CHCATF

  TITLE6:
CRAPIE

  TITLE7:
WALEYE

  TITLE8:
<<8>>

  TITLE9:
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  TITLEA:
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  TITLEB:
PHYTC

  TITLEC:
MACRC

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WATER

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<PCM>

  TITLEF:
PCM
```

```
 TITLEG:
CLAY

 TITLET:
TTIME

 00001 :
UUUUUUUUUU UUUUUUUUUU

 00002 :
 0.345E-01

 AREAT :
 0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451      0.451

 ALPHA :
 1.00        1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00     UUUUUUUUUU UUUUUUUUUU

 BACB  :
 0.590E-05  0.600E-05  0.100E-04

 BDINT :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 BDSLP :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 BLDC2 :
 0.170E-03  0.170E-03  0.170E-03  0.170E-03  0.170E-03  0.170E-03  0.170E-03  0.170E-03  0.170E-03  0.170E-03

 BMIN  :
 0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.0        0.0        0.0

 BTMAX :
 0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04  0.100E-04

 BTTIM :
 1.00        1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00       1.00

 CMAX  :
 1.00       0.100E-02  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  1.00       1.00       1.00

 CONCEN:
0.450       0.250       1.30       1.30       1.30      0.600E-01  0.600E-01  0.0        0.0        0.0        0.400      0.300
0.400E-05   0.0        0.400E-01  0.400E-01

 CSAT  :
0.250

 CYCLE :
 365.

 D     :
 1.00

 DELTA :
0.100

 E     :
0.300       0.300      0.700      0.700      0.700      0.700      0.700      0.300      0.300      0.300      0.300      0.300
```

EPA-287 (Cin.)
(4-76)

```
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0
0.300     0.300     0.700     0.700     0.700     0.700     0.700     0.300     0.300     0.300     0.300     0.300
0.0

 ELAM  :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0

 EN    :
0.0       0.0       0.0       0.0

 ERROR :
0.100E-02

 FAIRAT:
0.100E-07 0.100E-07 0.300E-03 0.300E-03 0.300E-03 0.300E-03 0.300E-03 1.00      1.00      1.00

 FECSWT:
 1.00     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0

 FMAX  :
0.600E-01  1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00      1.00

 HA    :
0.0       0.0       0.0       0.0

 HE    :
0.0       0.0       0.0       0.0

 HENRY :
0.541E-05

 TIMEAS:
 1.00

 KA    :
0.0       0.0       0.0       0.0

 KE    :
0.0       0.0       0.0       0.0

 KEIRAN:
0.250     0.250     0.250     0.250     0.250     0.250     0.250     0.250     0.250     0.250     0.250     0.250

 KCAL  :
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
DROPPED HEAD; BEGIN SECTIONS HERE
CENTER OF PAGE
TOP OF IMAGE AREA

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0.0        0.0        0.0        0.0

 KDEPTH:
0.400

 KDIFF :
0.444E-05

 KEFF  :
0.0        0.0        0.0        0.0

 KEC   :
 1.00

 KEED  :
0.250      0.250      0.250      0.250      0.250      0.100

 KEXCR :
0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03   1.00       1.00       1.00

 KH    :
0.0        0.0        0.0        0.0

 KMEAS :
0.0

 KMCPT :
0.200E-03  0.100E-03  0.100E-03  0.100E-03  0.860E-04  0.100E-03  0.110E-04  0.0        0.0        0.0        0.200E-04  0.200E-04

 KC    :
0.0        0.0        0.0        0.0

 KC2   :
 1.07       1.07       1.07       1.07       1.07       1.07       1.07       1.07       1.07       1.07

 KCH   :
0.0        0.0        0.0        0.0

 KF    :
0.0        0.0        0.0        0.0

 KEART :
0.100E+06  0.100E+05  0.100E+05  0.100E+05

 KFH   :
 1.00       1.00       1.00       1.00

 KBEST :
0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03  0.100E-03

 KS    :
 10.0       10.0       10.0

 KT    :
 1.00       1.00       1.00       1.00

 KIEME :
0.100E-01  0.100E-C1  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01   1.00       1.00       1.00

 KTE   :
```

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

EPA-287 (Cin.)
(4-76)

```
 1.00        1.00        1.00        1.00

 KTURB :
0.250       0.250       0.250       0.250       0.250       0.250

 LIFHIL:
UUUUUUUUUU

 MEIMAX:
0.400E-02   0.400E-02   0.400E-02

 MKG2  :
0.100E-01   0.100E-01   0.100E-01

 MMGI  :
2.00        2.00        2.00

 MOLCWT:
381.

 NUMB  :
0.0

 OCCND :
0.0         0.0         0.400E-01   0.0         0.900E-01   0.0          1.00       0.0         0.100E-01   0.0         0.0          1.07
0.0         0.0         0.200E-01   0.0         0.800E-01   0.0          1.00       0.0         0.100E-01   0.0         0.0          1.07
0.0         0.0         0.0         0.500E-01   0.600       0.600E-01    1.00       0.0         0.100E-01   0.0          1.07        1.07
0.0         0.0         0.0         0.200E-01   0.300        1.00        1.00       0.0         0.100E-01   0.0          1.07        1.07
0.0         0.900       0.0         0.0         0.250        1.00        1.00       0.0         0.100E-01   0.0          1.07       0.100E-01
0.0         0.800E-01   0.0         0.0         0.500E-01    1.00       0.0         0.0          1.00       0.0          1.07       0.0
0.0         0.100       0.0         0.0         0.0          1.00       0.0          1.00        1.00       0.0          1.07       0.100E-01
0.0         0.0         0.800E-01   0.0         0.0          1.00       0.0         0.100E-02    1.00       0.0          1.07       0.100E-01

 PARAMS:
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 1.00        1.00        1.00        1.00       0.541E-05    314.        14.8        96.0        1.00        365.       0.100E-02    1.00
 1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00       UUUUUUUUUU  UUUUUUUUUU  0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
 1.00        1.00        1.00        1.00        215.       0.100       0.450       0.250        1.30        1.30        1.30       0.600E-01
0.600E-01   0.0         0.0         0.0         0.400       0.300       0.400E-05   0.0         0.400E-01   0.400E-01    2.00        2.00
 2.00       0.170E-01   0.170E-01   0.170E-01    1.00        1.00        1.00       0.590E-05   0.600E-05   0.100E-04   0.400E-02   0.400E-02
0.400E-02    10.0        10.0        10.0        3.00        3.00        3.00        3.00        12.0        12.0        12.0        12.0
 1.00        1.00        1.00        1.00        298.        298.        298.        298.       0.100E-01   0.760       0.100       0.700
0.100       0.150       0.0         0.0         0.0         0.0         0.0         0.0         0.200       0.0         0.400       0.200
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.400E-01   0.900E-01   0.100       0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.400E-01   0.900E-01   0.100       0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.900E-01   0.100       0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.400E-01   0.200       0.350       0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.400E-01   0.900E-01   0.350       0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.900       0.800E-01   0.100       0.0         0.400E-01   0.200E-01   0.0         0.0         0.0         0.0         0.0         0.800E-01
0.0         0.0         0.500E-01   0.200E-01   0.0         0.0         0.0         0.0         0.900E-01   0.800E-01   0.600       0.300
0.250       0.500E-01   0.0         0.0         0.0         0.0         0.600E-01    1.00        1.00        1.00        1.00        1.00
 1.00        1.00        1.00        1.00        1.00       0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0          1.00       0.100E-02   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01    1.00        1.00        1.00
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0          1.07        1.07
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 1.07        1.07        1.07        1.07        1.07        1.07        1.07        1.07       0.100E-01   0.0         0.100E-01   0.100E-01
0.100E-01   0.100E-01   0.100E-01   0.0         0.0         0.0         0.451       0.451       0.451       0.451       0.451       0.451
0.451       0.451       0.451       0.451       0.100E-01   0.100E-01   0.100E-01    1.00        1.00        1.00       0.400       UUUUUUUUUU
UUUUUUUUUU  UUUUUUUUUU  0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.170E-03   0.170E-03   0.170E-03   0.170E-03   0.170E-03   0.170E-03   0.170E-03   0.170E-03   0.170E-03   0.170E-03    215.        35.0
 35.0        30.0        30.0        30.0        30.0        30.0        50.0        50.0        50.0        35.0        35.0       0.200E-03
0.100E-03   0.100E-03   0.100E-03   0.860E-04   0.100E-03   0.130E-04   0.0         0.0         0.0         0.200E-04   0.200E-04    1.00
 1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00        1.00       0.100E-04
0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.250
0.250       0.250       0.250       0.250       0.250       0.250       0.250       0.250       0.250       0.250       0.250       0.100
UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU  0.444E-05   0.345E-01   0.250       0.0          15.0        15.0        15.0        15.0        30.0
 30.0        30.0        30.0        1.00        1.00        1.00        1.00       0.300       0.300       0.300       0.300       0.300
0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300
0.300       0.300       0.300       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700
0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700
0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700
0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700       0.700
0.700       0.700       0.700       0.700       0.700       0.300       0.300       0.300       0.300       0.300       0.300       0.300
0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300
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0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.300
0.300       0.300       0.300       0.300       0.300       0.300       0.300       0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0          381.       0.100E+06   0.100E+05   0.100E+05   0.100E+05   0.100E-01   0.100E-01   0.100E-01   0.100E-01
0.100E-01   0.100E-01   0.100E-01    1.00        1.00        1.00       0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03
0.100E-03    1.00        1.00        1.00       0.200       0.200       0.200       0.200       0.200       0.200       0.200       0.200
0.200       0.200       0.500E-01   0.500E-01   0.150E-01   0.140       0.160       0.120       0.800E-01   0.0         0.0         0.0
0.100E-07   0.100E-07   0.300E-03   0.300E-03   0.300E-03   0.300E-03   0.300E-03    1.00        1.00        1.00       0.100E-04   0.100E-04
0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-03   0.100E-03   0.100E-03   0.100E-03
0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.400       0.400       0.400       0.400       0.400       0.400
0.400        1.00        1.00        1.00       0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.100E-03   0.0
0.0         0.0          2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00        2.00
 2.00        2.00       UUUUUUUUUU   40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0
 40.0        40.0        40.0        40.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0
 25.0        25.0        25.0        25.0        25.0        1.00       0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.500E-01   0.500E-01
0.500E-01   0.0         0.0         0.0         0.200       0.500E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01
0.100E-01   0.100E-01   0.300       0.500E-01    1.00       0.500       0.500       0.900       UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU  UUUUUUUUUU
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UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU
UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU
UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU
UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU
UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU
UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU UUUUUUUUUU

 RCRIC :
0.200      0.200      0.200      0.200      0.200      0.200      0.200      0.200      0.200      0.200

 RCRLW :
 215.

 RCFAT :
0.500E-01  0.500E-01  0.500E-01  0.500E-01  0.500E-01  0.500E-01  0.500E-01  0.0        0.0        0.0

 RCFRL :
 215.

 RFTRCE:
0.500E-01  0.500E-01  0.150E-01  0.140       0.160      0.120      0.800E-01  0.0        0.0        0.0

 RHMAX :
 12.0       12.0       12.0       12.0

 RHMIN :
 3.00       3.00       3.00       3.00

 RRATIC:
 298.      0.0        0.200      0.0        0.0        0.0        0.0        0.200      0.0        0.0        0.0        0.0
0.100E-01  0.0        0.0        0.400E-01  0.0        0.0        0.0        0.350      0.400E-01  0.0        0.0        0.0
0.760      0.0        0.0        0.900E-01  0.0        0.0        0.0        0.0        0.900E-01  0.0        0.0        0.0
0.100      0.0        0.0        0.100      0.400E-01  0.0        0.0        0.0        0.350      0.0        0.0        0.0
0.700      0.0        0.0        0.0        0.900E-01  0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.100      0.200      0.0        0.0        0.100      0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.150      0.0        0.0        0.0        0.0        0.900E-01  0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.400      0.0        0.0        0.0        0.100      0.400E-01  0.0        0.0        0.0        0.0        0.0

 RSIA  :
 1.00

 RSIR  :
 1.00

 C     :
0.400      0.400      0.400      0.400      0.400      0.400      0.400       1.00       1.00       1.00

 C10   :
 2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00       2.00
UUUUUUUUUU

 CI    :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0

 RAD   :
0.0        0.0        0.0        0.0

 RADIUS:
0.0        0.0        0.0        1.00       1.00       UUUUUUUUUU 0.0        0.450      0.400      0.170E-01  0.400E-02  12.0
0.0        0.0        0.0        1.00       1.00       0.0        0.0        0.250      0.300      0.170E-01  10.0       12.0
```

```
0.0         0.0         0.0         0.541E-05   1.00        0.0         0.0         1.30        0.400E-05   1.00        10.0        1.00
0.0         0.0         0.0          314.       1.00        0.0         0.0         1.30        0.0         1.00        10.0        1.00
0.0         0.0         0.0          14.8       1.00        0.0          1.00       1.30        0.400E-01   1.00        3.00        1.00
0.0         0.0         C.0          96.0       1.00        0.0          1.00       0.600E-01   0.400E-01   0.590E-05   3.00        1.00
0.0         0.0         0.0          1.00       1.00        0.0          1.00       0.600E-01    2.00       0.600E-05   3.00        298.
0.0         0.0         0.0          365.       1.00        0.0          1.00       0.0          2.00       0.100E-04   3.00        298.
0.0         0.0          1.00       0.100E-02   1.00        0.0          215.       0.0          2.00       0.400E-02   12.0        298.
0.0         0.0          1.00        1.00       UUUUUUUUUU  0.0         0.100       0.0         0.170E-01   0.400E-02   12.0        298.

 RMAX  :
0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04   0.100E-04

 SAFEA :
0.200       0.500E-C1   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.100E-01   0.300       0.500E-01
 1.00       0.5C0       0.500       0.900

 SHAPE :
0.541E-05    1.00       0.0         0.0          1.30       0.400E-05    1.00       10.0         1.00       0.100       0.200       0.0
 314.        1.00       0.0         0.0          1.30       0.0          1.00       10.0         1.00       0.700       0.0         0.0
 14.8        1.00       0.0          1.00        1.30       0.400E-01    1.00       3.00         1.00       0.100       0.400       0.400E-01
 96.0        1.00       0.0          1.00       0.600E-01   0.400E-01   0.590E-05   3.00         1.00       0.150       0.200       0.900E-01
 1.00        1.00       0.0          1.00       0.600E-01    2.00       0.600E-05   3.00         298.       0.0         0.0         0.100
 365.        1.00       0.0          1.00       0.0          2.00       0.100E-04   3.00         298.       0.0         0.0         0.0
0.100E-02    1.00       0.0          215.       0.0          2.00       0.400E-02   12.0         298.       0.0         0.0         0.0
 1.00       UUUUUUUUUU  0.0         0.100       0.0         0.170E-01   0.400E-02   12.0         298.       0.0         0.0         0.0
 1.00       UUUUUUUUUU  0.0         0.450       0.400       0.170E-01   0.400E-02   12.0        0.100E-01   0.0         0.0         0.0
 1.00        0.0        0.0         0.250       0.300       0.170E-01    10.0       12.0        0.760       0.0         0.0         0.0

 STEU  :
0.170E-C1   0.170E-C1   C.170E-01

 STTCM :
 1.00        1.00        1.00

 TCCND :
0.100E-01   0.451       0.100E-01 UUUUUUUUUU  0.0         0.170E-03    35.0       50.0        0.100E-03   1.00        1.00        0.100E-04
0.1C0E-01   0.451       C.100E-01 UUUUUUUUUU  0.0         0.170E-03    30.0       35.0        0.130E-04   1.00        1.00        0.100E-04
0.100E-01   0.451       0.100E-01  0.0        0.0         0.170E-03    30.0       35.0        0.0         1.00        1.00        0.100E-04
0.0         0.451        1.00      0.0        0.0         0.170E-03    30.0       0.200E-03   0.0         1.00        0.100E-04   0.100E-04
0.0         0.451        1.00      0.0        0.170E-03   0.170E-03    30.0       0.100E-03   0.0         1.00        0.100E-04   0.100E-04
0.0         0.451        1.00      0.0        0.170E-03   0.170E-03    30.0       0.100E-03   0.200E-04   1.00        0.100E-04   0.100E-04
0.451       0.451       0.400      0.0        0.170E-03    215.        50.0       0.100E-03   0.200E-04   1.00        0.100E-04   0.100E-04
0.451       0.451       UUUUUUUUUU 0.0        0.170E-03    35.0        50.0       0.860E-04    1.00       1.00        0.100E-04   0.250

 TCCPT :
298.        298.        298.        298.

 TCFIT :
35.0        35.0        30.0        30.0        30.0        30.0        30.0        50.0        50.0        50.0        35.0        35.0

 TMAX  :
40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0        40.0
40.0

 TOPT  :
25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0        25.0
25.0

 TEPAX :
30.0        30.0        30.0        30.0
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EPA-287 (Cin.)
(4-76)

```
 TEMIN :
 15.0       15.0       15.0       15.0

 VEEN  :
 96.0

 VFUDGE:
 1.00

 VH2C  :
 14.8

 VICM  :
 314.

 W     :
0.1C0E-01  0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.900      0.0
0.9C0E-01
0.760      0.0        C.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.800E-01  0.800E-01
0.800E-01
0.100      C.200      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.100      0.0
0.600
0.700      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.300
0.100      0.400      0.400E-01  0.400E-01  0.0        0.400E-01  0.400E-01  0.0        0.0        0.0        0.400E-01  0.500E-01
C.250
0.150      0.200      0.900E-01  0.900E-01  0.900E-01  0.200      0.900E-01  0.0        0.0        0.0        0.200E-01  0.200E-01
0.500E-01
0.0        0.0        0.100      0.100      0.100      0.350      0.350      0.0        0.0        0.0        0.0        0.0
0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0
0.0        0.0        C.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0

 EFFEN :
0.1C0E-01  0.0        0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.100E-01  0.0        0.0        0.0

 WMIX  :
 1.00       1.00       1.00

 DEBUGS:
F F F F F F F F F F
F F F F F F F F F

 DISLCD:
F

 DISRAT:
F

 DPRCCS:
F F F F F F F F F F
F F F F F F

 DTIME :
F
```

PAGE NUMBER

EPA-287 (Cin.)
(4-76)

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD; BEGIN SECTIONS HERE
BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS

```
 ICE    :
T T T F F F F F F F
F T

 NUPIC :
    12        2        15        15        15        15        15         0         0         0
    12       15        12         0         2         2        24        24        24        24
     0        0         0         0         0         0         0         0         0         0
     0        0         3         0         0         0         0         0

 STEP   :
    60

 SWITCH:
     0

 TFIRST:
     1

 TLAST  :
   3650

 CLAY   :
0.500      0.500      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 CLAYT  :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 DC2    :
 11.5       10.4       3.90       3.00       7.90       15.4       12.8       5.00       3.30       2.80       4.60       3.50
 7.20       4.10       4.40       3.10       3.90       5.00       7.50       9.10       9.70       12.8       14.5       12.0
0.0        0.0        0.0        0.0        0.0        0.0

 DC2T   :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 FISH1  :
 1.67       1.63       1.65       1.68       1.78       1.87       1.96       2.06       2.09       2.09       2.07       2.00
 1.93       1.81       1.75      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 FISH1T:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 FISH2  :
 2.20       2.15       2.18       2.22       2.35       2.47       2.59       2.72       2.77       2.77       2.74       2.65
 2.55       2.40       2.30      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 FISH2T:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

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0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH3 :
 1.13      1.10      1.12      1.14      1.21      1.27      1.33      1.40      1.42      1.42      1.41      1.36
 1.31      1.23      1.18      0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH3T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH4 :
0.714     0.697     0.706     0.721     0.762     0.802     0.841     0.882     0.898     0.898     0.889     0.858
0.826     0.778     0.745     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH4T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH5 :
0.238     0.232     0.235     0.240     0.254     0.267     0.280     0.294     0.299     0.299     0.296     0.286
0.275     0.259     0.248     0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH5T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH6 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH6T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH7 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH7T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH8 :
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
0.0       0.0       0.0       0.0       0.0       0.0
 FISH8T:
0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
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EPA-287 (Cin.)
(4-76)

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 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PCM    :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PCPT   :
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  LOAD38:
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  LDG    :

  LDI    :

  MACBC  :
 0.134      0.130      0.132      0.139      0.151      0.166      0.180      0.191      0.198      0.200      0.195      0.185
 0.172      0.157      0.144      0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  MACPOT:
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PCLAY  :
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 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PFISH1:
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 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PFISH2:
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PFISH3:
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PFISH4:
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0

  PFISH5:
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PFISH6:
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PFISH7:
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PFISH8:
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PFCM  :
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 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PH    :
 7.80     7.30     7.00     7.10     7.30     8.40     8.30     7.50     7.90     7.60     7.90     7.80
 8.10     7.80     7.50     7.20     7.50     7.50     7.80     7.90     7.90     8.30     7.90     7.60
 0.0      0.0      0.0      0.0      0.0      0.0

 PHT   :
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PHYTC :
 0.114    0.342    0.231    0.570    1.76     0.164    0.346    0.268    0.620    0.970    1.05     0.990
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PHYTCT:
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PMACPC:
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PCP   :
 1.00     1.00     0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PCMT  :
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0

 PPHYTC:
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
 0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0      0.0
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0.0         0.0         0.0         0.0         0.0         0.0

 FECM  :
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0.0         0.0         0.0         0.0         0.0         0.0

 FWATER:
0.405E-07   0.150E-08   0.500E-10   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
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0.0         0.0         0.0         0.0         0.0         0.0

 FWBUGS:
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 FZCOPI:
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 SCIAR :
 34.8        44.8        82.7        121.        140.        176.        252.        264.        456.        313.        491.        584.
 472.        491.        388.        581.        547.        352.        349.        437.        313.        428.        275.        206.
 166.        172.        91.8        77.7        55.8        31.9

 TEMP  :
0.200       0.800       0.800        3.60        4.80        6.80        6.50        20.3        15.9        22.2        22.0        25.8
 27.4        26.8        25.0        22.4        23.1        18.1        14.5        11.2        9.40        2.90       0.800        1.00
0.0         0.0         0.0         0.0         0.0         0.0

 TEMPI :
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 WATER :
0.760E+05   0.190E+06   0.800E+06   0.630E+06   0.440E+06   0.280E+06   0.280E+06   0.430E+06   0.540E+06   0.290E+06   0.300E+06   0.160E+06
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 WBUGS :
0.200E-02   0.200E-02   0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 WBUGSI:
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0

 WIND  :
 5.00        4.50        4.50        4.00        3.84        3.84        3.44        3.44        2.82        2.36        3.58        3.31
 2.50        2.64        2.24        2.79        2.68        3.80        3.40        3.26        3.44        3.44        3.53        4.00
0.0         0.0         0.0         0.0         0.0         0.0

 WINDI :
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0         0.0
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TOP OF IMAGE AREA

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0.0        0.0        0.0        0.0        0.0        0.0

 WIND  :
 5.00       4.50       4.50       4.00       3.84       3.84       3.44       3.44       2.82       2.36       3.58       3.31
 2.50       2.64       2.24       2.79       2.68       3.80       3.40       3.26       3.44       3.44       3.53       4.00
0.0        0.0        0.0        0.0        0.0        0.0

 WINDT :
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 ZCCPI :
0.100E-08  0.870E-02  0.580E-02  0.150E-01  0.450E-01  0.420E-02  0.880E-02  0.680E-02  0.160E-01  0.250E-01  0.270E-01  0.250E-01
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0

 ZCCPIT:
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0        0.0
0.0        0.0        0.0        0.0        0.0        0.0
6 Yes?
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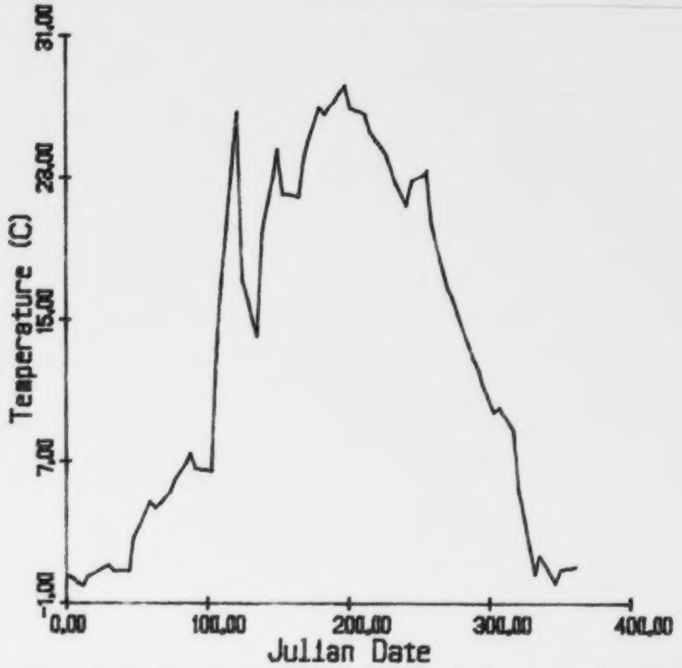

Figure D.1. Temperature loadings used in simulation of Coralville Reservoir, Iowa.

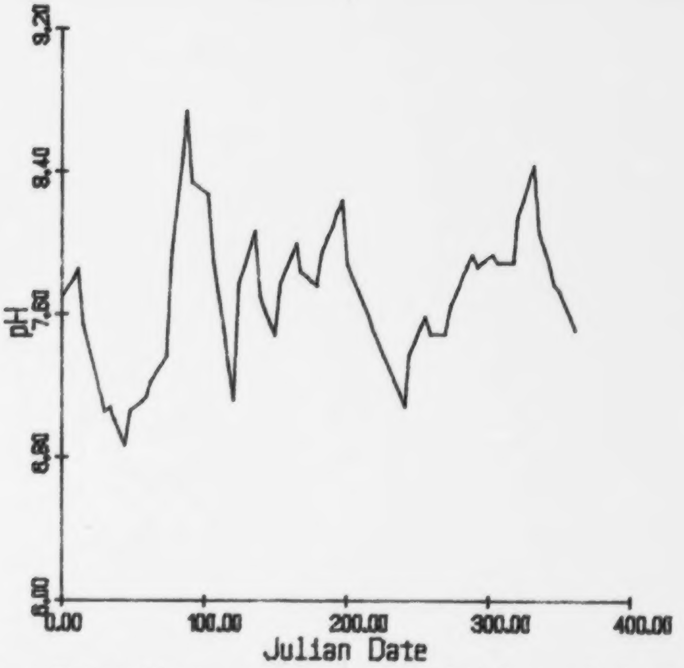

Figure D.2. pH loadings used in simulation of Coralville Reservoir, Iowa.

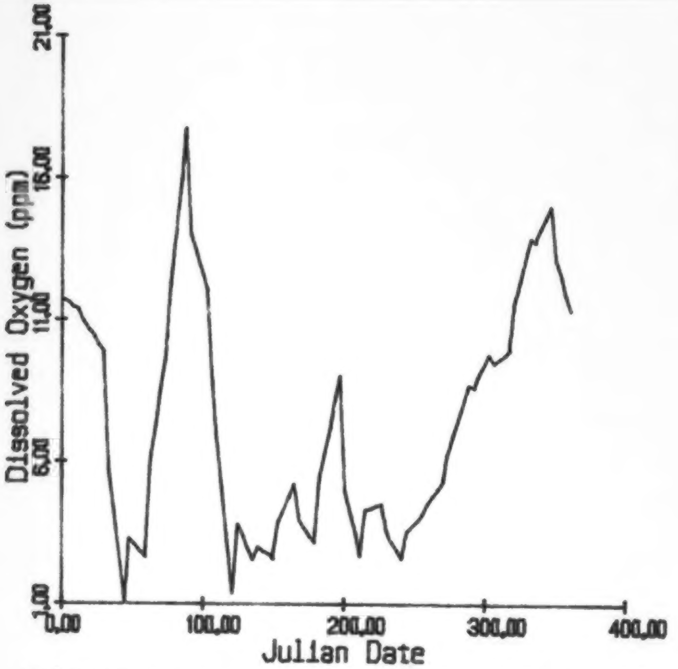

Figure D.3. Dissolved oxygen loadings used in simulation of Coralville Reservoir, Iowa.

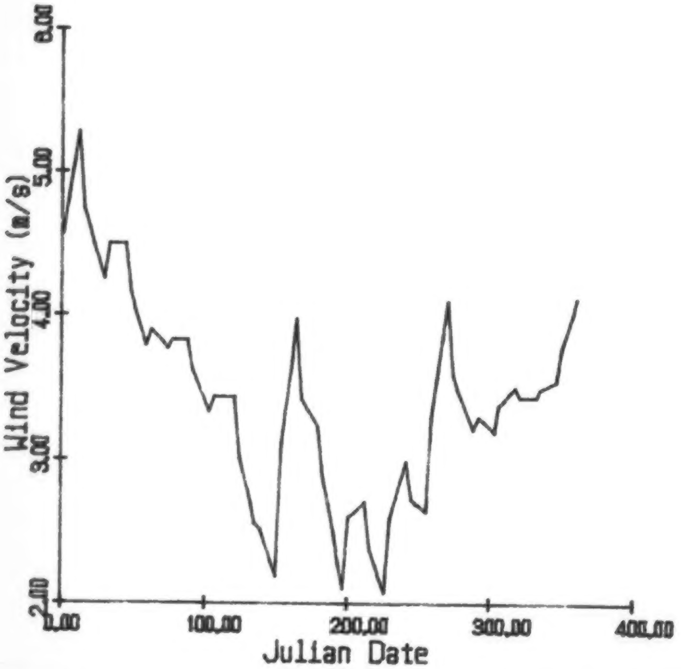

Figure D.4. Wind loadings used in simulation of Coralville Reservoir, Iowa.

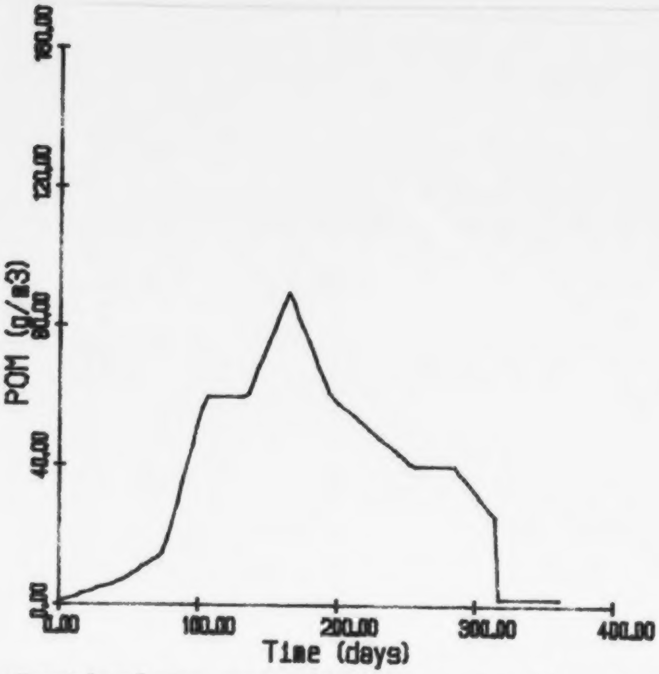

Figure D.5. Particulate organic matter loadings used in simulation of Coralville Reservoir, Iowa.

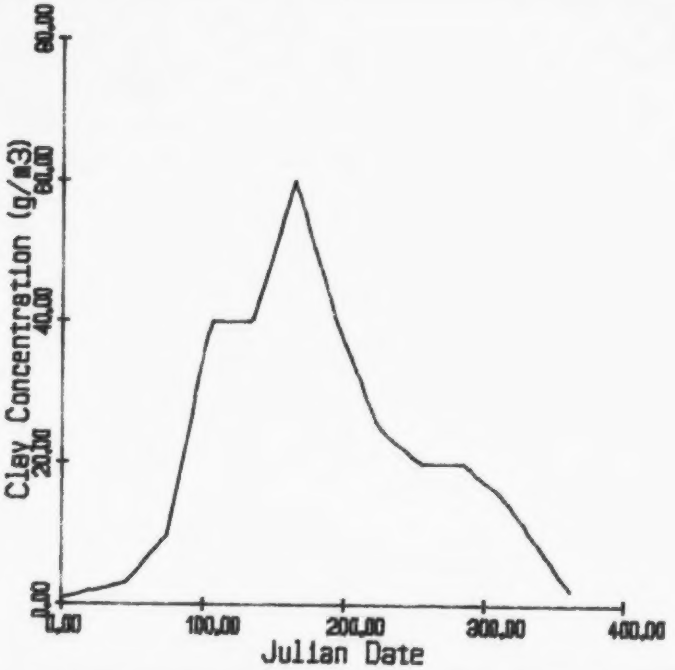

Figure D.6. Clay loadings used in simulation of Coralville Reservoir, Iowa.

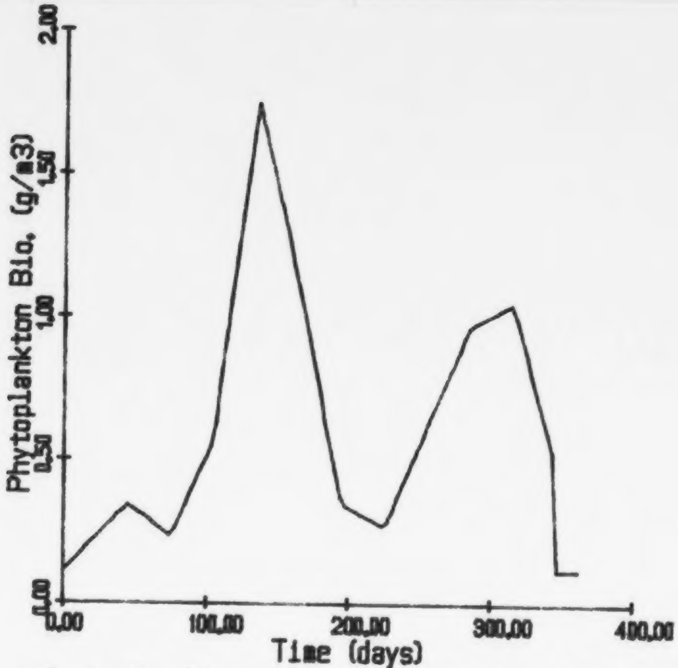

Figure D.7. Phytoplankton biomass used in simulation of Coralville Reservoir, Iowa.

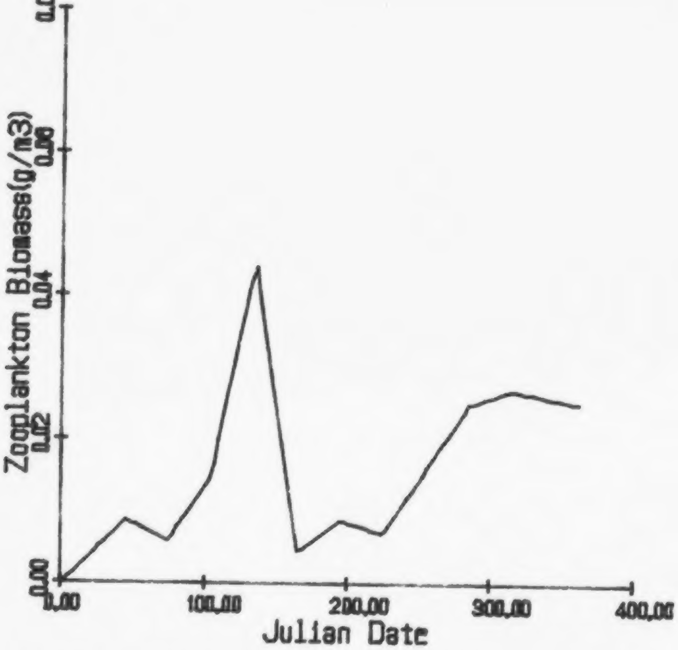

Figure D.8. Zooplankton biomass used in simulation of Coralville Reservoir, Iowa.

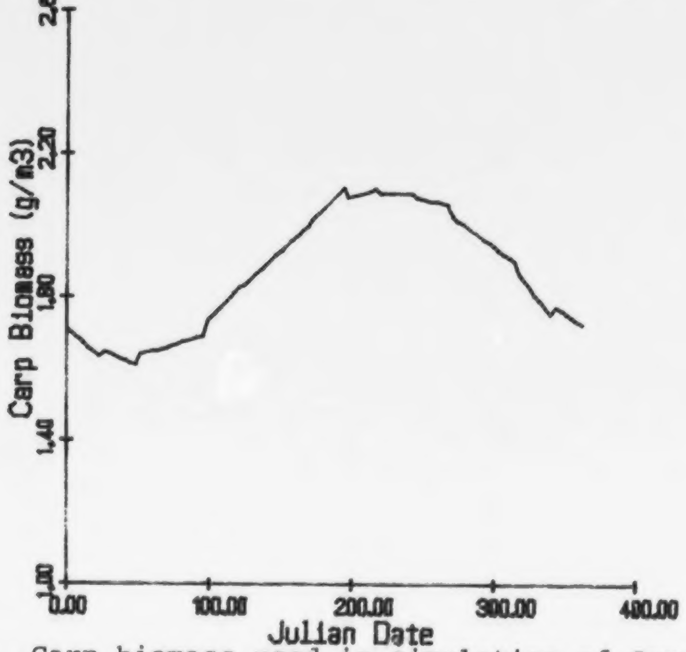

Figure D.9. Carp biomass used in simulation of Coralville Reservoir, Iowa.

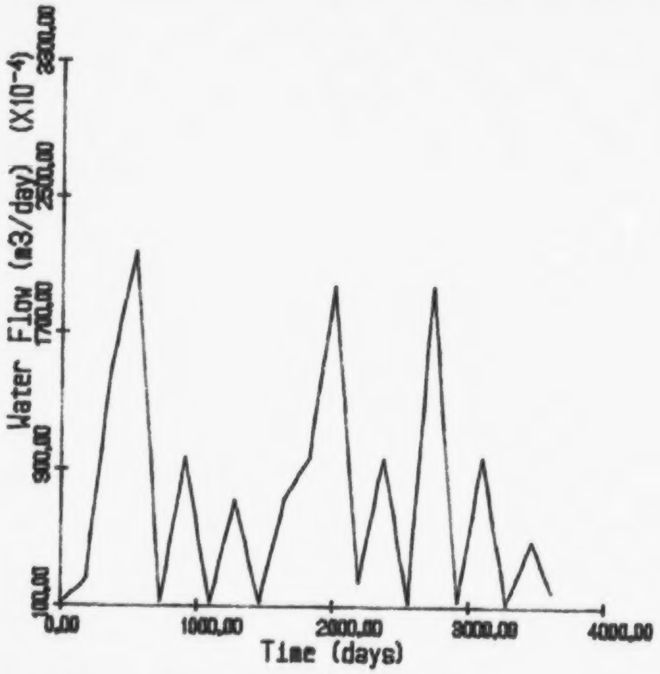

Figure D.10. Water flow loadings used in simulation of Coralville Reservoir, Iowa.

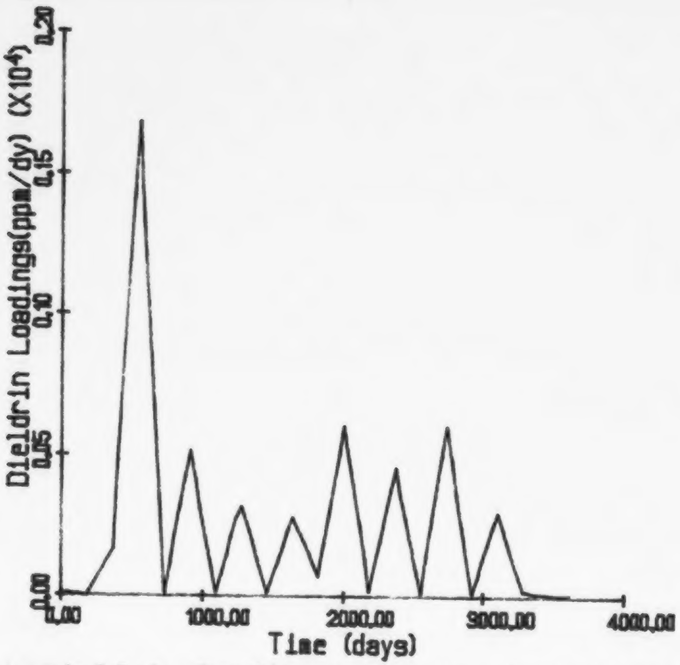

Figure D.11. Dieldrin loadings used in simulation of Coralville Reservoir, Iowa.

GLOSSARY OF PARAMETERS AND VARIABLES

A:	activity coefficient for microbial degradation (unitless) (pp. 32, 33)
ALPHA:	extinction coefficient for site water at each wavelength (l/cm) (pp. 17, 20)
BACB:	microbial biomass (g/m^3) (p. 39)
BCIRC:	concentration of TOM that passes through the gills in the blood (g/m^3 day) (p. 42)
BDINT:	coefficient for biodeposition (unitless) (p. 47)
BDSLP:	coefficient for biodeposition (unitless) (p. 47)
BIO:	biomass of each organism (g/m^3) (pp. 42, 45)
BIODEP:	rate of production of pseudofeces (g/g day) (p. 47)
BLDO2:	coefficient for oxygen capacity of blood (g O2/g blood) (p. 43)
BMIN:	the prey concentration at which predator begins feeding (g/m^3) (pp. 46, 47)
BTMAX:	maximum rate of biotransformation (g/g biomass day) (p. 49)
BTRANS:	rate of biotransformation of TOM by higher organisms (g/m^3 day) (p. 48)
BTTIM:	number of days required to reach full metabolic capacity (day) (p. 49)
CMAX:	maximum rate of ingestion (g/g day) (p. 45)
CONCEN:	concentration of toxic organic material (g/m^3) (p. 7)
CONS:	rate of change of TOM in organism as a result of ingestion, defecation, and excretion (g TOM/m^3 day) (p. 44)
CPTWO:	rate of ingestion of TOM by predator (g TOM ingested/m^3 day) (p. 47)
CRS:	rate of biomass loss due to respiration (g/m^3 day) (pp. 42, 43, 48)
CTWO:	total rate of consumption by each organism (g/m^3 day) (p. 42, 45)
D:	median depth of water (cm) (pp. 17, 18)

DEF1: rate of defecation of TOM (g/m^3 day) (p. 47)

DEPTH: depth of water (m) (p. 38)

DIR: difference in TOM concentrations in water and blood (g TOM/m^3 day) (pp. 43, 44)

DOCOR: reduction of microbial degradation due to suboptimal oxygen levels (unitless) (p. 33)

DOMIN: minimum value of oxygen reduction under anaerobic conditions (unitless) (pp. 33, 35)

DO2: dissolved oxygen concentration (g/m^3) (pp. 35, 43, 46)

DPHLIM: depth at which wind energy is unimportant for mixing effect on microbial degradation (m) (p. 38)

DTWO: total rate of defecation by each organism (g/m^3 day) (p. 42)

E: percentage of TOM in prey that is egested (unitless) (pp. 47, 48)

EFFEN: coefficient for diffusivity of TOM through gill membrane (unitless) (p. 44)

ELAM: molar extinction coefficient for TOM at each wavelength (l/mole cm) (p. 17)

EN: activation energy for effect of temperature (cal/mole) (p. 7)

EX: rate of excretion of TOM by each organism (g/m^3 day) (p. 48)

EXPT: time of exposure to TOM (days) (p. 39)

EXTRA: amount of TOM not in solution (g/m^3) (p. 31)

FIL: rate of filtering (g/g day) (p. 47)

FRACD: fraction of irradiance that is direct at each wavelength (unitless) (p. 17)

FRACS: fraction of irradiance that is indirect at each wavelength (unitless) (p. 17)

GILSRP: rate of sorption by gills (g/m^3 day) (pp. 41, 44)

HA: concentration of Bronsted acid (g/m^3) (p. 7)

HB: concentration of Bronsted base (g/m^3) (p. 7)

HENRY: Henry's Law constant (atm cm^3/mol) (pp. 26, 27)

HYDR: rate of hydrolysis (g/m^3 day) (p. 7)

IIMEAS: observed light intensity (photons/cm^2) (pp. 20, 21)

IITOT: total incident light (photons/cm^2) (p. 20)

INT: width of wavelength interval (nm) (p. 17)

KA: rate constant for Bronsted acid catalysis (1/days)

	(pp. 7, 11; sum of wavelength-specific, direct photolysis rate constants (l/day) (p. 16)
KB:	rate constant for Bronsted base catalysis (l/days) (pp. 7, 11)
KBTRAN:	half-saturation coefficient for biotransformation (g TOM/m^3) (p. 49)
KCAL:	rate constant to account for colloidal, metal-ion, and phase-transfer catalysis (l/days) (pp. 7, 12)
KDEPTH:	constant relating wind energy to depth (p. 38)
KEFF:	rate of radical initiation reaction (l/day) (p. 15)
KEQ:	equilibrium dissociation constant (not used) (p. 20)
KEXCR:	proportionality coefficient for excretion as a function of respiration (unitless) (p. 48)
KGAS:	gas-phase mass transfer coefficient (cm/hr) (pp. 24, 26)
KH:	acid-catalyzed rate constant (l/M days) (pp. 7, 9)
KLEXPT:	correction factor for volatilization (unitless) (p. 24)
KLIQ:	liquid-phase mass transfer coefficient (cm/hr) (pp. 24, 28)
KMEAS:	rate constant for sensitized photolysis (l/day) (pp. 20, 21)
KO:	uncatalyzed rate constant (l/days) (pp. 7, 9, 11)
KOH:	base-catalyzed rate constant (l/M days) (pp. 7, 9, 11)
KO2:	saturation coefficient for oxygen limitation of ingestion (g/m^3) (p. 46)
KP:	rate of reaction between TOM and alkoxy and peroxy radicals (l/day) (p. 15)
KPART:	octanol-water partition coefficient (unitless) (p. 40)
KPH:	adaptive constant for pH effect on microbial degradation (unitless) (p. 40)
KRESP:	proportionality constant for respiration as a function of metabolism (unitless) (p. 42)
KS:	half-saturation constant for microbial metabolism (g/m^3) (p. 32)
KSEN:	empirical rate constant for sensitized photolysis (l/day) (pp. 16, 20)
KT:	rate of competing reaction between two radicals re-

	sulting in non-radical products (1/day) (p. 15)
KTEMP:	coefficient relating respiration rate to temperature (1/°C) (p. 42)
KTP:	adaptive constant for effect of temperature on microbial degradation (unitless) (pp. 37, 38)
LAM:	wavelength (nm) (p. 17)
LD:	effective direct underwater path length for irradiance (cm) (p. 17)
LIM:	reduction in ingestion rate due to low prey concentration (unitless) (pp. 45, 46)
LOAD:	concentration of each carrier (g/m^3) (pp. 40, 41)
LS:	effective diffuse underwater path length for irradiance (cm) (p. 17)
MAX:	maximum rate of biotransformation under ambient environmental conditions (g/g biomass day) (p. 49)
METCAP:	percent metabolic capacity for degradation of TOM (unitless) (p. 49)
METMAX:	maximum rate of microbial metabolism (1/day) (pp. 32, 33)
MKO2:	half-saturation constant for effect of oxygen on microbial degradation (g/m^3) (pp. 33, 35)
MMGT:	microbial generation time under optimal conditions (days) (p. 39)
MMET:	rate of degradation due to microbial metabolism (g/m^3 day) (p. 32)
NEWAMT:	equilibrium concentration for each carrier (ppm) (p. 40)
NORM:	rate of gill sorption normalized for all organisms (unitless) (p. 44)
OLDAMT:	concentration of TOM in carrier not affected by adsorption (g/m^3) (p. 41)
OXID:	rate of oxidation (g/m^3 day) (p. 15)
O2RESP:	coefficient relating oxygen uptake to respiration (g O2/g biomass) (pp. 42, 43)
PCBLD:	percent blood (g blood/g biomass) (p. 43)
PCBLW:	blood:water partition coefficient, (p. 43)
PCFBL:	fat:blood partition coefficient, (p. 43)
pH:	ambient pH, (pp. 7, 13, 36)
PHCOR:	reduction factor for microbial degradation due to pH (unitless) (pp. 33, 35, 37)

PHMAX: critically high pH for microbial degradation, (pp. 36, 37)

PHMIN: critically low pH for microbial degradation, (pp. 36, 37)

PHOT: rate of photolysis (g/m^3 day) (p. 16)

PSIA: direct photolysis quantum yield for the TOM (unitless) (pp. 16, 17)

PSIB: sensitized photolysis quantum yield for the TOM (unitless) (p. 16)

Q: half-saturation constant for feeding (g/m^3) (pp. 45-47)

Q10: rate of change per 10°C temperature change (unitless) (p. 46)

RAD: concentration of radical initiator present, (p. 15)

RE: Reynolds Number (unitless) (p. 30)

RMAX: respiration rate at starvation (g/g day) (p. 42)

SAREA: percentage of TOM at surface of carrier (unitless) (p. 40)

SOLU: amount of TOM in solution (g/m^3) (p. 31)

SOLUB: solubility (ppm) (pp. 26, 31)

SORP: routine for calculating TOM concentration due to sorption, (pp. 40, 41)

STRU: structural activity factor for microbial degradation (unitless) (pp. 39, 40)

STTOM: Julian date of introduction of TOM, (pp. 39, 49)

T: water temperature (°C) (= TEMP) (p. 46)

TADPT: effective biomass of TOM-degrading microflora (g/m^3) (pp. 32, 39)

TCOPT: temperature at which rate constant was obtained (°K) (p. 7)

TCORR: Arrhenius temperature correction factor (unitless) (p. 7)

TEMP: ambient temperature (°C) (pp. 7, 26, 37, 42)

TIME: Julian date in simulation, (p. 39)

TMAX: maximum temperature at which process will occur (°C) (p. 46)

TMIX: reduction factor for effect of suboptimal mixing on microbial degradation (unitless) (pp. 33, 38)

TOPT: optimum temperature (°C) (pp. 42, 46)

TOTPST: total concentration of TOM at site (g/m^3) (p. 40)

TPCOR: reduction factor for effect of nonoptimal temperature on microbial degradation (unitless) (pp. 37, 38)

TPMAX: critically high temperature for microbial degradation (°C) (p. 37)

TRBRED: reduction factor in filtering rate due to high turbidity (unitless) (p. 47)

TRED: reduction factor for non-optimal temperature (unitless) (pp. 46, 49)

VBEN: molal volume of benzene (cm^3/mol) (p. 28)

VH2O: molal volume of water (cm^3/mol) (p. 26)

VOLAT: rate of volatilization (moles/m^2 hr) (p. 24)

VPRESS: vapor pressure (Hg) (p. 26)

VTOM: molal volume of TOM (cm^3/mol) (pp. 26-28)

W: preference of predator for prey (unitless) (p. 45)

WCIRC: amount of TOM in water that passes through gill (g TOM/m^3 water processed day) (pp. 43, 44)

WINDV: wind velocity (m/sec) (pp. 26, 38)

WMIX: windspeed at one-half maximum stirring effect (m/sec) (p. 38)

INDEX

Adaptation, 39
Aerobic, 35
Anaerobic, 35
Animals, 3
Aromatic Ring, 35
Arrhenius Energy Equation, 7
Attenuation Coefficients, 18
Atrazine, 8, 12, 22, 27, 31

Benthic, 45
Benzene, 28
Bioaccumulation, 53, 54
Biochemical Oxygen Demand, 33
Biodeposition, 47
Biotransformation, 48
Blood, 42
Bluegills, 64
Bronsted Acid, 7, 12
Bronsted Base, 7, 12
BTRANS, 4, 48

Calibration, 57
Carbaryl, 8, 14, 22, 27, 31
Carnivores, 45
Carp, 59
Channel Catfish, 65
Clay, 4, 62
Colloidal Catalysis, 12
Columbia National Fisheries
  Research Laboratory, 61
Common Block, 76, 81
Compound-Specific, 51
CONS, 3, 44
Consumption, 44
Coralville Reservoir, 63

Data Requirements, 51
DEBUG, 71
DEF, 3, 44
Defecation, 44
Depth of Water, 18
Diagnostic, 51
Dieldrin, 27, 31, 63
Diffusivity, 29, 44
DISPLAY, 75
Dissolved Phase, 58, 61, 64, 66
Driving Variables, 54, 75
DUMP, 76

EDIT, 68
Electrolyte Concentration, 8
Evaluative, 51
EX, 3
EXAMS, 1
Excretion, 44, 48

Fat, 42, 48
Field Verification, 57
File Units, 79
Filter-Feeders, 45
Fish Ponds, 58
Floating Organic Matter (FOM), 4

Gas-Phase, 26
Gill Sorption, 41
GILSRP, 3, 41
Glossary, 156

HELP, 77
Henry's Law Constant, 26
Hydrolysis, 7, 51
HYDR, 4, 51

Ingestion, 44
Iowa, 63
Israel, 58

Large-Mouth Bass, 63, 65
Lipophyllic, 41, 48
Liquid-Phase, 28
LOADS, 4
LOGON, 68

Malathion, 8, 12, 15, 22, 27, 31
Metal-ion Catalysis, 13
Methoxychlor, 8, 9, 10, 22, 27

Microbial, 55
Microbial Degradation, 52
Microbial Metabolism, 32
Missouri, 61
Mixing, 38
MMET, 4
Molal Volume, 26
Molecular Volume, 26
MORT, 3
MSUM, 4

Octanol-Water Partition Coefficient, 40
Organism-Specific, 54
Output, 5
OXID, 4, 15
Oxidation, 15, 52
Oxygen, 46

Parameter File, 83
Parameter Index, 80
Parameters, 51
Parathion, 8, 9, 15, 22, 27, 31, 58
Particulate Organic Matter (POM), 4, 62
Pentachlorophenol, 8, 9, 10, 22, 27, 31, 61
pH, 8, 11, 13
PHOT, 4, 16
Photolysis, 16, 52
Phytoplankton, 62
Plants, 4
PLOT, 73
Ponds, 61
PRINT, 70
Process Name, 72
Pseudofeces, 45, 47

QUIT, 78

Respiration, 43

Sedimentation, 66
Sediments, 61
Sensitized Photolysis, 20
SERATRA, 2
Silver Carp, 60
Simazine, 12
Site-Specific, 53
Solar Intensity, 18
SOLU, 4, 31
Solubility, 31
Solution, 31, 52
SORP, 4, 40
Sorption, 40, 53
SPOO, 79, 83
START, 69
State Variables, 2
S-triazine, 12
Structural Activity, 39

TABULATE, 73
Tape, 82
Temperature, 37, 46
Tilapia, 60

Uncertainties, 57
Universal Gas Constant, 7

Validity, 57
Verification, 57
VOLAT, 4, 24
Volatilization, 24, 52

Water (Dissolved Phase), 4
Whitman Two-Film, 25
Wind, 26, 28, 30

Zooplankton, 59, 62

2,4-D, 8, 9, 11, 14, 22, 27, 31